FY 2000 ANNUAL OPERATING PLAN

HYDROGEN PROGRAM

Prepared for

U. S. DEPARTMENT OF ENERGY
OFFICE OF POWER TECHNOLOGIES

by

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1.0 INTRODUCTION

This document is the Annual Operating Plan of the Department of Energy (DOE), Hydrogen Research and Development (R&D) Program. It serves to provide the DOE's management and program participants with the plans for fiscal year 2000 (FY 2000). This document contains general information on the Hydrogen R&D Program and its goals, project summaries listing the planned activities for FY 2000 (including Gantt charts with expected key milestones), significant results and accomplishments from 1999, and listings of publications, patents, and national recognition achieved by the Principal Investigators.

The Hydrogen Program is part of the Office of Power Delivery Systems within the Office of Power Technologies (OPT), which is in turn within the Office of Energy Efficiency and Renewable Energy. The organization of the Hydrogen Program is detailed in Chapter 2. The Program includes three focus areas: A) Research and Development of Critical Component Technologies (production, storage, and utilization), B) Technology Validation, and C) Analysis and Outreach.

The DOE Hydrogen R&D Program supports the Matsunaga Hydrogen Research, Development, and Demonstration Act of 1990 (P.L. 101-566), the Energy Policy Act of 1992 (P.L. 102-486) Section 2026, and the Hydrogen Future Act of 1996 (P.L. 104-271), and addresses the energy and environmental benefits of hydrogen. The Program put forth by the DOE has been designed to develop, in collaboration with industry as well as with other Federal entities, the technologies necessary to safely produce, store, transport, and utilize hydrogen as an energy carrier; to illustrate the energy and environmental benefits to the public sector; and to initiate the transition strategy which can bring these technologies successfully to the marketplace.

1.1 Implementing the Twenty-Year Vision

Hydrogen allows for both the increased use of renewable energy and CO_2 sequestration technologies that help to reduce CO_2 emissions. It can replace polluting fuels and result in near-zero urban pollutants being emitted into the atmosphere. With this in mind, the DOE Hydrogen program laid out its Twenty-Year Vision in the Strategic Plan:

In the next twenty years, concerns about global climate change and energy security will create the platform for the penetration of hydrogen into several niche markets. Ultimately, hydrogen and electricity will come from sustainable renewable energy resources, but fossil fuels will be a significant transitional resource during this period. The growth of fuel cell technology will provide a base for the establishment of the hydrogen option into both transportation and electricity supply markets.

Since the strategic plan was written in 1998, the Hydrogen Program has helped to advance hydrogen technologies. The Twenty-Year vision given in the document was aimed towards the long-term development of renewable based hydrogen technologies. In the interim, fossil fuels are to be a transitional resource. This is significant, because the technologies that use fossil fuels and that enable hydrogen in both the fuel infrastructure and vehicle technologies exist today, and can meet near term markets. Furthermore, there are **no technical showstoppers** to implementing a near-term hydrogen fuel infrastructure for direct hydrogen fuel cell vehicles. Fundamentally, the technologies required are available but there are engineering development needs as well as codes and standards and other institutional issues to resolve.

A key driver for hydrogen vehicles is the California Zero Emissions Vehicle (ZEV) mandate. The ZEV mandate requires that by the year 2005, 10% of the total vehicles sold will be zero emission vehicles.

Under the mandate, the number of "pure ZEVs" (i.e., hydrogen fuel cell vehicles or battery electric vehicles) will be 1% of the total vehicle market or about 10,000 hydrogen fuel cell vehicles.

In the near term, fuel cell vehicles will most likely be used in fleet applications to accommodate higher vehicle costs as well as fueling, operation, and maintenance requirements. Hydrogen-fueled buses will also be utilized in a few urban areas and as well as by some very progressive transit agencies that have compressed natural gas (CNG) fueling facilities. Under the federal Energy Policy Act (EPACT), alternative fuel vehicles (AFV) fleets may provide the most direct opportunities in the near-term. DOE's overall mission is to replace 10% of petroleum-based motor fuels by the year 2000 and 30% by the year 2010. EPACT mandates federal, state, and alternative fuel provider fleets to purchase AFVs.

1.2 DOE Hydrogen Program Strategic Approach

The DOE Hydrogen Research and Development Program's mission is to conduct research and engineering development in the areas of hydrogen production, storage, and utilization for the purpose of making hydrogen a cost-effective energy carrier for utility, buildings, and transportation applications. The program is now looking to prepare hydrogen technologies to meet California's ZEV mandate requirements, and the push for Distributed Generation.

The program intends to expand the short-term applications of hydrogen through partnerships with industry that will allow improvements in efficiency, decrease emissions, and lower the cost of hydrogen production. Projects are being undertaken with fuel cell manufacturers to develop hydrogen based electricity storage and generation systems that will enhance the introduction and production of distributed systems. The program also aims to develop codes and standards and safe systems to facilitate the creation of a hydrogen infrastructure. Systems will be developed that are cost-effective and safe for use in hydrogen vehicles in urban non-attainment areas, in addition to the creation of on-board hydrogen storage systems. The program also aims to lower the cost of technologies that produce hydrogen directly from sunlight and water.

1.2.1 Production Goals

If fuel cell vehicles are going to be competitive on the open market, an infrastructure for the generation and distribution of hydrogen must be established. To compete with other energy carriers, such as electricity, natural gas, and petroleum, the cost of generating hydrogen must come down. A system for distributing the fuel must also be commercially available.

- **Improving the efficiency and lowering the cost of fossil based and biomass-based hydrogen production processes to $6-$8/ MMBtu**

Initially, hydrogen utilized in fuel cells will be produced from natural gas. The competing option will be to burn the natural gas/hydrogen blends in combustion turbines or internal combustion engines. To make fuel cells competitive with respect to the combustion options, the cost differential between hydrogen and natural gas must be minimized. Toward this aim, the goal of $6-$8/ MMBtu production cost of fossil-based and biomass-based hydrogen was established. In addition, in order to support the transportation market, the Program has set a goal of $12-$15/MMBtu (which is approximately 60-75 cents per gallon of gasoline before taxes, based on a fuel-cell vehicle with an equivalent of about 82mpg) for the cost of producing pressurized hydrogen at the refueling station.

Hydrogen can also be produced by the gasification of dedicated biomass crops for approximately $6-$8/ MMBtu. By adding CO_2 sequestration, both the natural gas and biomass strategies can be augmented. Hydrogen can be produced by these technologies and delivered to a vehicle less expensively than gasoline on a mile per gallon equivalent basis when compared with today's 28 miles per gallon efficiencies.

- **Advancing emission-free and renewable-based hydrogen production technologies towards commercial viability, with a target cost of $10-$15/ MMBtu**

In order to advance the mission relating to technologies that produce hydrogen from sunlight and water, the Hydrogen Program will pursue long-term electrolytic, photoelectrochemical, and photobiological research and development. The program has set a goal of producing electrolyzers at efficiencies greater than 92% for less than $300/ kW.

1.2.2 Storage and Utilization Goals

Hydrogen vehicles will not be cost effective unless storage is priced competitively. Market forces, particularly cost, will be the key driver bringing fuel cell vehicles to compliance with California's ZEV mandate. To facilitate the development of a hydrogen infrastructure to support fuel cell vehicles and ultimately electricity generation from hydrogen, the goals below were developed.

- **Demonstrating safe and cost-effective storage systems for use in stationary distributed electricity generation applications, and for on-board and stationary applications in urban non-attainment areas**

A major improvement in hydrogen storage performance will be necessary for hydrogen to gain acceptance as an effective energy carrier. With intensive interest in mobile applications and as the amount of intermittent renewable electricity increases, hydrogen storage becomes an essential element of these systems. Current technology permits the physical storage, transport, and delivery of hydrogen, in gaseous or liquid form, in tanks and pipeline systems. These physical storage systems have been used in various stationary and mobile demonstrations, but the issues of safety and energy consumption require the development of advanced storage concepts based on advanced materials for physical storage and chemical storage mediums. The program aims to develop storage that is greater than 5% hydrogen by weight for on-board vehicle storage.

- **Developing fuel cell and reversible fuel cell technologies as an efficient low-cost means of converting hydrogen into electric power**

In order to develop a hydrogen infrastructure, the end-use technologies must be developed and matured. Here, the primary technology is the fuel cell. In order for fuel cells to be the "work horse" hydrogen utilization tool, several technical hurdles must be overcome. Fuel cells must be run on hydrogen directly to prevent CO_2 emissions; fuel cell efficiencies must be increased and their cost must be lowered to make them competitive; and reversibly electrolyzer/fuel cell modules must be developed that can enable substantial reductions in overall system costs. The Program aims to produce PEM fuel cells that cost less than $300/kW. In addition, the Program is striving toward reversible fuel cells having a round-trip efficiency of 70%, and a cost of less than $600/kW.

1.2.3 Technology Validation Goals

This focus area concentrates on validating nearer term technologies against a series of cost, performance, and safety objectives. This can include the integration of any combination of production, storage, transport, and utilization technologies, and is performed in collaboration with industry. These projects will help to facilitate hydrogen technologies' establishment as a viable application and ensure competitiveness with other technologies. Through the Technology Validation Program, DOE's Hydrogen Program will promote direct hydrogen fuel cell vehicles that meet the demands of California's ZEV mandate.

- **The goal of the Technology Validation is to support industry in the verification and demonstration of hydrogen systems in the utility and transportation sectors.**

Technology validation projects integrate components of novel and advanced technology into test-bed energy systems to evaluate their potential. Parallel development of advanced fossil-based and renewable-based production systems, as well as current and advanced storage and utilization technologies, will provide a set of critical experiences to industry as they evaluate the introduction of the technologies into niche markets.

The strategy of the technology validation is within the Technology Validation Plan. The Program will achieve the above goal by operating under the following objectives:

1. Obtain industry participation through competitive solicitations for mid-term development and proof-of-concept testing

2. Integrate renewable energy resources with hydrogen storage in remote, distributed power scenarios

3. Test the viability of hydrogen production, storage, and refueling stations within several clean clusters

4. Evaluate remote and residential "total" energy PEM fuel cell systems

5. Develop hydrogen-based operating experience acceptable to meet safety codes and standards.

1.2.4 Environmental Goals

The generation and consumption of energy is the largest single source of air pollution in the United States. Electricity produced from fossil fuels results in one-third of all carbon-based emissions. The oil-dependent transportation sector contributes another third. To cut emissions and reduce the effects of harmful urban pollutants, such as NO_x, SO_x, and CO, there must be a shift away from fossil fuel-based energy and an increasing dependence on renewable sources of energy. In response, the Hydrogen Program has set forth the goals of reducing emissions in urban non-attainment areas, and reducing global greenhouse gas emissions. The goals are to displace 1.87 million tons of carbon by 2010 and 13.45 million tons of carbon by 2020. Emissions are to be reduced by 51,900 tons/year of NO_x, 390,500 tons/year of CO, and 45.6 million tons/year of CO_2 by 2020.

1.2.5 Policy, Planning, and Analysis Goals

Analysis and technology transfer incorporates many of the activities formerly grouped under the titles of Systems Analysis and Integration, Technology Transfer, and Industry and Educational Outreach. This includes the identification and definition of research opportunities for hydrogen as an energy carrier through system and infrastructure evaluations and analyses. Analysis will be used to determine the economic feasibility of various scenarios through the calculation of life cycle costs of individual production, storage, transport, and end-use technologies, as well as overall systems. Projects such as technical brochures, fact sheets, and exhibits will all be evaluated and presented to the Program. As set forth in the Strategic Plan the goals of Policy, Planning, and Analysis include:

- **Ensuring that Federal R&D investments in hydrogen production, storage, distribution, and end-use technologies will provide the maximum value added to national strategic goals including global greenhouse emission mitigation**

The goal of supplying significant amounts of renewable hydrogen to the electricity supply and transportation markets in 20 to 30 years cannot be achieved with current budgets unless they are highly leveraged with other Federal programs and with industry. The key planning and analysis issue for the Program is how to define and maximize its "value-added" to the national and global transition to renewable energy.

- **Identifying and evaluating key market segments and market entry conditions for hydrogen utilization in transportation and in electricity generation at distributed and remote locations**

In order for policy makers to make rational decisions regarding the utilization of hydrogen, it is necessary that they receive the pertinent information and recommendations from the Program and industry. These recommendations must evolve from data developed from the development and validation components of the Program, and must incorporate reasonable and thorough systems analysis of hydrogen integrated pathways.

- **Developing and applying metrics to measure the Program's contribution to attaining national strategic energy goals and market share in key segments**

It is necessary for the program to develop a database that will incorporate cost, performance, reliability, lifetime, and other key characteristics for hydrogen technologies to contribute to national strategic energy objectives and compete in key market segments.

1.2.6 Outreach and Coordination Goals

In California, the public must also be aware of the air quality improvements that result from the use fuel cell vehicles and the ZEV mandate. The Program conducts various industry outreach, public outreach, and international activities including efforts in three major areas: workshops and conferences, exhibits and trade shows, and publications. These outreach and technology transfer activities span the entire program structure. The goal of the outreach is:

- **Conduct outreach and coordination to develop informed constituencies in the industrial and public sectors as part of a strategy to accelerate the commercialization of renewable hydrogen technologies.**

For hydrogen to act as an energy carrier, the public must be informed of the technology. The public must be made aware of the economic and environmental benefits of hydrogen technologies, the level of safety associated with hydrogen technologies, and industry's impressive safety record producing and using large quantities of hydrogen.

2.0 TECHNICAL ORGANIZATION

2.1 Approach

The techniques employed by the Program emphasize state-of-the-art methods for: (1) genetic engineering to develop biological systems that can produce hydrogen directly from water or carbon-rich substrates such as the syngas produced from gasification of biomass; (2) engineering and manufacturing of high performance semiconductors that will directly convert photons (light energy) to hydrogen by splitting water; (3) developing newer high-efficiency methods to thermally break down fossil feedstock and biomass to produce high purity hydrogen; and (4) producing of engineered materials for high performance storage systems such as carbon nanotubes and fibers that can adsorb large volumes of hydrogen.

2.2 Objectives

The objectives of the Hydrogen Program are to develop the critical technologies for hydrogen systems and support a vision of a sustainable energy future that includes hydrogen and electricity as the energy carriers. The accomplishment of these objectives will lead to improved energy use and efficiency, lower environmental emissions, and fuel use flexibility.

The Program supports the following activities: (1) developing and integrating the technology base for producing hydrogen using fossil and renewable sources; (2) developing advanced materials and delivery systems for storage and transport options; (3) evaluating safety and reliability issues associated with utilization technologies; (4) performing technical and economic analyses on component technologies and processes; and (5) demonstrating hydrogen technologies within integrated energy systems, with strong industry collaboration.

2.3 Hydrogen Program Organization

The Hydrogen Program incorporates technical and management assistance provided by key program participants to guide the Program's management and direction, which is established by a DOE Headquarters Management Team. The Hydrogen Technical Advisory Panel (HTAP), National Hydrogen Association (NHA), National Renewable Energy Laboratory (NREL), Sandia National Laboratories (SNL), and other Program participants submit input to the Program through both formal and informal mechanisms. These groups provide DOE with recommendations on the implementation and conduct of the Program, multi-year planning and resource allocation between technical and analytical issues. Additionally, technical review teams provide DOE with insights on the progress and direction of research and development, and a means by which researchers and industry can exchange information. Technology Road Maps, outlining the path over the next five years toward meeting these objectives, are recent additions to the Program guidance.

The development of broad-based hydrogen energy systems necessitates interaction and cooperation among a number of crosscutting research and development projects and technologies within the Department and other Federal agencies. The Hydrogen Program is charged with the responsibility (via the Matsunaga and Hydrogen Future Act) to provide this Federal coordination role. DOE has entered into several collaborations in R&D and validation with the DOE Offices of Transportation Technologies, Building Technologies, Fossil Energy, and Science as well as the Defense Advanced Research Programs Agency, Defense Conversions Program, and the National Aeronautics and Space Administration (NASA).

The Program goals and objectives are met by funding projects within universities, National Laboratories, and industry; monitoring the performance of projects; conducting an Annual Peer Review of all projects; reviewing all technical and programmatic plans with HTAP; circulating monthly program status reports to all of the program principal investigators (PIs) to facilitate communication; and disseminating hydrogen information through publications, participation in technical meetings, and substantive contacts with stakeholders. The activities funded by the Program are classified into three focused areas: a) Core R&D, b) Technology Validation, and c) Analysis and Technology Transfer. As a result of increased Program funding, many activities that have proven successful R&D phases, are now moving into the technology validation area.

2.4 Management Structure

The Hydrogen Program is managed by the Department of Energy, with technical oversight and management assistance provided by NREL and SNL. DOE provides technical and programmatic guidance, sets budgetary marks and establishes programmatic goals. The Program organization is shown in Figure 2.1. Headquarters activities are lead by the Hydrogen Program Management Team.

The DOE, Golden Field Office is responsible for coordination of the Program's cost-shared collaborative agreements. This includes project and financial management, and the issuing, coordinating, and evaluating of the Hydrogen Program's solicitations.

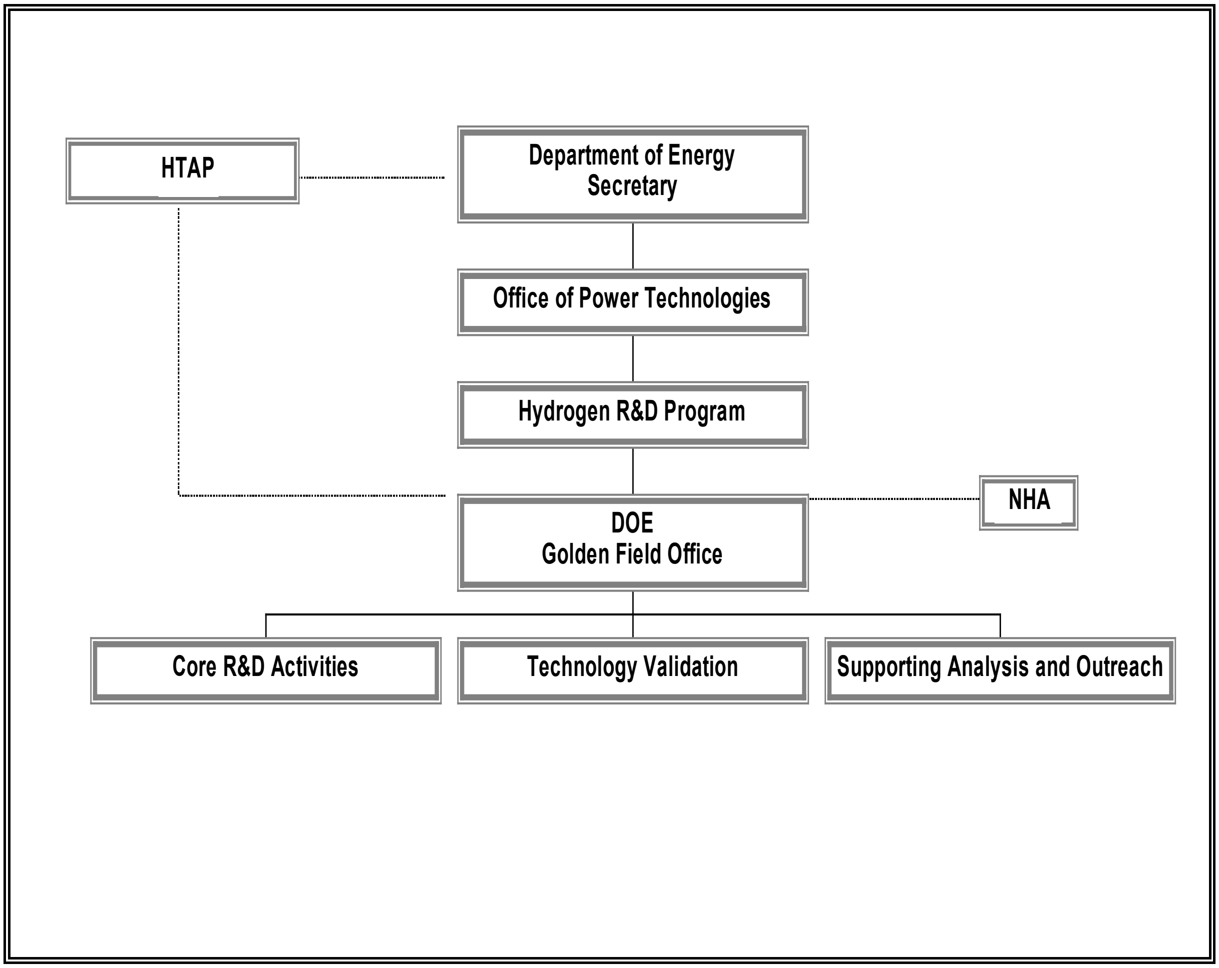
A group of technical managers, made up of scientists and engineers within the program also provide technical guidance and coordinate within the areas of thermal production, photoelectrolytic and photobiological production, storage, and utilization hydrogen R&D.

The NREL and SNL Program Offices participate in DOE planning efforts through technical reviews of proposals, annual peer review, and strategic planning meetings. Additionally, the NREL Program Office plans and executes the HTAP meetings, and produces and distributes all publications associated with the Panel and its subcommittees. The SNL Program Office plans and executes the Remote Power and Nevada fueling station activities.

HTAP, as mandated by the Matsunaga Act and amended by the Hydrogen Future Act, advises DOE management in carrying out the Program. The panel members, nominated by the Secretary of Energy, represent industry, universities, financial and environmental organizations, and address issues such as developing market-sensitive transition paths from near-term to longer-term programmatic objectives.

NHA, comprised of industry members, participates in safety, codes and standards activities related to the safe use of hydrogen. Widespread hydrogen use will require that safety be intrinsic to all processes and systems to ensure the public's complete confidence in hydrogen as a fuel. NHA is taking a lead in pushing forward codes and standards for the handling of hydrogen. In addition, there is an effort to have international codes and standards committees treat hydrogen as a stand-alone gas.

Figure 2.1
DOE Hydrogen Program Organization



3.0 PROGRAM ELEMENTS

3.1 R&D on Hydrogen Production, Storage and Utilization

The objective for this area is to develop critical cost-effective technologies by conducting research and development in the areas of production, storage, transport, and utilization. The work is conducted at universities, national labs, and industry as shown in the table accompanying each section.

3.1.1 Hydrogen Production Research Projects

The FY 2000 hydrogen production projects, summarized in Table 3.1 and 3.2, are broken up into four categories. These include fossil-based and biomass-based production, and electrolytic and photobiological processes. Separation techniques are included in “fossil-based production”, and photoelectrochemical processes are included in the “electrolytic category”.

Table 3.1
Fossil/Biomass Based Production

Goal: Improve the efficiency and lower the cost of fossil-based and biomass-based hydrogen production processes to $6-$8/MMBtu

Category	Project	Researchers
Fossil-Based Production	Hydrogen Manufacturing Using Plasma Reformers	Massachusetts Institute of Technology
	High Yield Production of Hydrogen and Carbon from Natural Gas	Idaho National Engineering and Environmental Laboratory
	Hydrogen Production from Diesel Fuels for use with Fuel Cell Systems	Argonne National Laboratory
	Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor	National Renewable Energy Laboratory
	Separation Membrane Development	Savannah River Technology Center
	Production of H_2 by Superadiabatic Decomposition of Hydrogen Sulfide	Institute of Gas Technology
	Thermocatalytic CO_2 – Free Production of Hydrogen from Hydrocarbon Fuels	Florida Solar Energy Center
	Sorption Enhanced Reaction Process for Production of Hydrogen (H_2-SER)	Air Products and Chemicals, Inc.
	Engineering Development of Ceramic Membrane Reactor Systems for converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels	Air Products and Chemicals, Inc.
	Novel Catalytic Fuel Reforming	InnovaTek
Biomass-Based Production	Hydrogen Production from High-Moisture Content Biomass in Supercritical Water	University of Hawaii
	Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming	National Renewable Energy Laboratory
	Biomass Pyrolysis for Hydrogen Production	Jet Propulsion Laboratory
	Modeling of the Supercritical Water Pyrolysis Process	Combustion Systems, Inc.

FOSSIL-BASED PRODUCTION

Hydrogen Manufacturing Using Plasma Reformers - Massachusetts Institute of Technology (MIT)

Manufacturing of hydrogen from natural gas, biofuels and other hydrocarbons, is needed for a variety of applications. Plasma technology could provide important improvements in reforming hydrocarbon fuels for the production of hydrogen-rich gas and facilitates use in a wide range of applications. The plasma conditions (high temperatures and a high degree of ionization) can be used to accelerate thermodynamically favorable chemical reactions without a catalyst or provide the energy required for endothermic reforming processes. Plasma reformers can provide a number of advantages:

- Economic operation in small to medium size units
- operation with a broad range of fuels, including natural gas and biofuels
- decreased problems of catalyst sensitivity and deterioration
- compactness and low weight (due to high power density)
- minimal cost (simple electrodes and power supplies)
- high conversion efficiencies

Two types of plasma reformers are being investigated. One is a conventional plasmatron using a DC-arc plasma. The other is a low power plasmatron which MIT has recently developed. Use of this device makes it possible to greatly reduce the specific electrical energy consumption. This reduction more than compensates for the increased energy loss due to increased exothermic energy release of the reforming process.

Hydrogen Manufacturing Using Plasma Reformers
Massachusetts Institute of Technology (MIT)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimization of new plasma reformer						
Develop heat regeneration with new plasma reformer		◆				
Develop metallica based heat exchanger				◆		
Develop ceramic honeycomb heat exchanger					◆	
Increased Range of Operation						
Increase power with conventional plasmatron		◆				
Increase power with new plasma reformer			◆			
Decrease power with new plasma reformer				◆		
Improved Reactor						
Design system		◆				
Optimize fuel injection			◆			
Optimize air injection				◆		
Develop thermal shielding					◆	
Pilot Plant						
Design plant based on conventional plasmatron				◆		
Design pilot plant with new plasma reformer						

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Task 1: Optimization of novel plasmatron configurations

The use of heat regeneration to preheat the air and/or the fuel will be tested. Preheating should decrease the electrical power required to bring the air and fuel to process temperature. It should be possible to decrease the specific energy consumption further. MIT is estimating that the specific electrical energy consumption with methane will be less than 5 MJ/kg H_2. This value is a factor of 3 lower than that obtained with the conventional plasmatron.

Task 2: Increased range of operation

For higher hydrogen production rates operation, the conventional plasmatron may be superior to the novel plasmatron configuration. Experiments with the conventional plasmatron will continue in order to determine the regimes where the conventional plasmatron may be superior to the novel plasmatron configuration.

Operation of the novel plasmatron configuration with diesel fuel (for the Alaskan fuel-cell project) will be investigated. The plasmatron electrical power will be increased to about 250-500 W from the 50-100 W of proof-of-principle device achieved during FY99.

Task 3: Improved reactor

The novel plasmatron configuration needs to be integrated into a system with a reaction extension region (a reactor downstream from the plasma and the fuel injection point), a heat exchanger, and various catalytic regions (steam reforming, and high and low temperature water-shifting). Sulfur poisoning of the catalyst will be determined.

Task 4: Pilot plant

A pilot plant for the generation of hydrogen at an appropriate throughput will be designed. Issues of lifetime and reliability will be addressed. A smaller unit with the novel plasmatron will be designed and constructed. Costing of the hydrogen with this new type of reformer will be evaluated.

High Yield Production of Hydrogen and Carbon from Natural Gas – Idaho National Engineering and Environmental Laboratory (INEEL)

Currently, most hydrogen is produced by steam reforming or partial oxidation. When natural gas is reformed by these processes, the carbon is converted to CO_2. Plasma thermal reforming of natural gas results in the carbon being isolated in solid form thus avoiding the potential cost of sequestering CO_2 if this should be required in the future. INEEL has patented technology for the plasma thermal conversion of natural gas. One process converts natural gas to acetylene and hydrogen with minimal production of solid carbon. Modification of the conditions utilized in this process results in the deeper conversion of natural gas to hydrogen and solid carbon.

This program will demonstrate the integrated efficient thermal conversion of methane to hydrogen, purification of the hydrogen, and utilization of the purified hydrogen in a PEM fuel cell. Because of the high degree of urgency in development of viable moderate scale hydrogen production methods to meet the geographically diverse market for transportation and distributed power applications, emphasis will be placed on the early technical validation of the integrated production/purification/fuel cell utilization. This preliminary validation will occur prior to complete optimization of the individual steps.

As fuel cells require a high degree of hydrogen purity, early efforts will include evaluation of technology for efficient separation of byproduct solid carbon from the hydrogen and removal of other impurities. It is presumed that cyclone separation plus a final filtration will be the most effective process for carbon removal. It is also presumed that membrane separation will be the most acceptable technology for removal of the other impurities. Conventional state-of-the-art Proton Exchange Membrane (PEM) fuel cell technology will be included in the technology validation effort. Its industrial CRADA partner, DCH Technology, Inc., will assist INEEL in this part of the effort.

As part of this effort, a commercialization plan will be developed. The lead in this effort will be taken by DCH.

High Yield Production of Hydrogen and Carbon from Natural Gas
Idaho National Engineering and Environmental Laboratory (INEEL)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Plasma Parametric Studies						
Complete plasma parametric studies	◆					
Hydrogen/ Carbon Separation and Hydrogen Analysis						
Complete method for hydrogen/ carbon separation	◆					
Preliminary Commercialization Plan						
Create a commercialization plan		◆				
Fuel Cell Selection						
Select fuel cell	◆					
Hydrogen Purification						
Select a purification system			◆			
Demonstration System Design and Construction						
Design and construct demonstration system			◆			
Initial Integrated Demonstration						
Demonstrate integrated system			◆			

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Task 1: Plasma Parametric Studies

This initial parametric study will not be exhaustive but will define satisfactory operating conditions for the initial demonstration of integrated hydrogen production, purification, and operation of the fuel cell. The plasma reactor will be modified as required to allow satisfactory conversion of methane to hydrogen and solid carbon. Once a satisfactory reactor configuration is achieved, the following parameters will be investigated: residence time, gas flow rates (both methane and plasma gases) and ratios, operating pressure, and power level.

This study will define operating characteristics for the initial integrated demonstration and will provide preliminary data on product stream purity and specific energy requirements. This preliminary data will be evaluated and supplied to its industrial CRADA partner and also to NREL for a preliminary comparison of the INEEL hydrogen production technology with other technologies.

Task 2: Hydrogen/Carbon Separation and Hydrogen Analysis

Methods for separation of the co-produced carbon will be conducted during the parametric study of Task 1. It is presumed that this separation will require a cyclone in combination with a finishing filter. Gas compositions including trace contaminants in the product gas will also be determined during Task 1.

Task 3: Preliminary Commercialization Plan

DCH Technology, Inc. with assistance from INEEL will create a commercialization plan that identifies the optimum market entry strategy for the INEEL technology in the context of the existing industrial requirements and future hydrogen energy opportunities. This includes a top-level integration plan for a complete hydrogen energy pathway. This includes safety assessment, storage, and possible hydrogen liquefaction. DCH will have CryoFuels Systems, Inc. on the initial commercialization team and others may be added. Solicitation of additional CRADA partners for the continuing effort is a part of this task.

Task 4: Fuel Cell Selection

DCH Technology, Inc. will conduct a survey of fuel cell providers and compare available PEM fuel cells. In consultation with DOE and INEEL, DCH will select the fuel cell power and define specifications for the fuel cell to be used in this demonstration program. Specifications for hydrogen requirements will be included. Efforts will be made to find a CRADA partner to provide the fuel cell to be used in the demonstration program.

Task 5: Hydrogen Purification (if funding permits)

Based on the studies of Task 1, a purification system will be selected in consultation with vendors. It is presumed that a commercially available membrane purification system will be optimal. The purification equipment will be procured and its performance evaluated. Conditions to produce the required hydrogen purity at the required hydrogen feed rate will be determined. Independent variables include upstream and downstream hydrogen pressure, separator configuration, discard gas rate, and feed gas composition. Dependent variables include purified gas composition and purified gas flow rate.

Task 6: Demonstration System Design and Construction (if funding permits)
In consultation with DOE and DCH, INEEL will complete design and construction of the integrated demonstration system (including hydrogen production, compression, purification, storage, and fuel cell operation).

Task 7: Initial Integrated Demonstration (if funding permits)

Following shakedown of the system, operation of all components in an integrated mode will be demonstrated. As the plasma reactor can produce hydrogen far in excess of that required by a 10kW fuel cell, the plasma reactor can be operated in an intermittent manner while allowing continuous operation of the fuel cell.

Hydrogen Production from Diesel Fuels for use with Fuel Cell Systems - Argonne National Laboratory

Task 1: Autothermal Reforming

This task supports the development of a 5 kW(e) fuel cell power plant demonstration work being conducted at Analytic Power Inc. Electric power will be generated by fuel cells, where the fuel cells will operate on hydrogen produced from diesel reforming. Argonne National Laboratory has developed a novel autothermal reforming catalyst and reforming process that has been shown to achieve the desired reaction at lower temperatures and without coking. Under this task Argonne National Laboratory will provide to Analytic Power the catalyst material for their reforming reactor. Necessary technical assistance will be provided to ensure that the operating conditions are suitable for the catalyst and for enhancing the hydrogen yields.

Task 2: Diesel Reforming in Micro-reactors

This task will be conducted to determine the operating conditions for the catalytic autothermal reforming of diesel and the long-term stability of the catalyst. These studies will be conducted in a micro-reactor apparatus – where the feeds consisting of vaporized fuel, steam, and air, will be passed over a 12-mm diameter reactor, and a tube furnace will be used to maintain the reactor and catalyst at the desired temperature.

Subtask 2.1: Long-Term Test of POX Catalyst
A long term test reactor will be built to evaluate the performance of the partial oxidation reforming catalyst under the operating conditions of diesel reforming. The reactor will be kept in a tube furnace with appropriate feeds of diesel, air, and steam passed over the catalyst. The catalyst temperature and the product gas will be analyzed during this period to determine if the catalyst deactivates. If performance

Hydrogen Production from Diesel Fuels for use with Fuel Cell Systems - Argonne National Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Autothermal Reforming at Analytic Power						
Deliver catalyst to Northwest Power		◆				
Deliver catalyst to Analytic Power		◆				
Test processor with ANL catalyst			◆			
Diesel Reforming in Microreactors						
Determine sulfur tolerance of reforming catalyst (200h)			◆			
Complete 1000 test of POX catalyst				◆		
Demonstrate <2% CO from diesel reforming				◆		
Deliver shift and PrOx catalyst to Analytic Power					◆	
Sulfur Removal From Liquid Fuel						
Identify sulfur sorption materials for testing					◆	
Reforming of synthetic diesel						
Demonstrate feasibility in microreactor			◆			

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degrades, as reflected by a loss in hydrogen yield, the cause(s) will be identified. Because of the high sulfur content of diesel fuel, the sulfur tolerance of the autothermal reforming catalyst will be determined in a reactor system dedicated to sulfur testing. This information is important to Northwest Power and Analytic Power.

Subtask 2.2 Reforming and CO Reduction
The reforming of hydrocarbons produces a large amount of carbon monoxide as a byproduct. Carbon monoxide is a poison for the polymer electrolyte fuel cell and therefore must be converted to carbon dioxide or removed before the reformate gas can be fed to the polymer electrolyte fuel cell. Catalysts will be tested in an apparatus consisting of an autothermal reformer, a water-gas shift reactor, and a preferential oxidation (PrOx) reactor. The water-gas shift reactor converts the carbon monoxide in the product from the first reactor into more hydrogen via the water-gas shift reaction ($CO + H_2O = CO_2 + H_2$). The PrOx reactor removes remaining CO to <100 PPM by reacting it with oxygen. The next generation shift and PrOx catalysts developed and tested in this apparatus will be tested in a 5 kW(e) fuel processor by Analytic Power. The objective of this subtask is to demonstrate that the combination of autothermal reforming and CO reduction can produce sufficient hydrogen while maintaining the carbon monoxide levels to under 100 PPM.

Task 3: Sulfur Removal from Liquid Diesel

Diesel fuels contain sulfur, which is a poison for many catalysts in the fuel processor and the fuel cell electrocatalyst. The petrochemical industry takes out the sulfur by the hydrodesulfurization process, one that is too complex to be applicable for remote fuel processing and fuel cell applications. Argonne National Laboratory has done some preliminary studies to investigate the absorption/adsorption of the sulfated species in gasoline onto solid substrates. This task will study various candidate materials and their ability to capture sulfur, to determine the feasibility of using this technique. If this process is found to be capable of reducing the sulfur to levels where the fuel processing catalysts are not easily poisoned, it will simplify the fuel processor design considerably. If the reforming catalyst can tolerate small quantities of sulfur, then the reforming process converts the sulfur into hydrogen sulfide, which is much more easily removed from the reformate stream by zinc oxide beds. Sulfur removal from liquid fuel is of particular interest to Northwest Power.

Task 4: Reforming of Synthetic Diesel

Synthetic fuels, such as those produced by the cobalt-based Fischer-Tropsch process, have the potential for use as a substitute for diesel. These fuels are much cleaner than diesel derived from crude oil in that they are sulfur-free and contain very little metals. The absence of these contaminants makes them easier to reform for fuel cell applications. These synthetic fuels are much more uniform in their hydrocarbon content than petroleum-derived fuels, and the hydrocarbon components are 99% straight-chained paraffins. Further, the composition of these fuels can be tailored to benefit higher hydrogen yields.

This task will undertake to study the reformability of synthetic diesel produced by Syntroleum Corporation, to determine the operating conditions and hydrogen yields achievable. This study will be conducted in a micro-reactor apparatus.

Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor - National Renewable Energy Laboratory (NREL)

The basis of this concept is the high temperature thermal dissociation of methane in a solar heated aerosol flow reactor. Methane is dissociated to carbon black and hydrogen in the following reaction:

$$CH_4 \rightarrow C + 2H_2 \quad \Delta H_{1600K} = 75 \text{ kJ/mole}$$

This reaction was experimentally demonstrated in 1978, was shown to be fast, and could be carried to 100% completion at temperatures greater than 1815^{o}C. The reactor consisted of an electrically heated aerosol reaction chamber. A small amount of carbon black was introduced to serve as a radiation-absorbing target to initiate the pyrolytic reaction. Once started, the carbon produced continued to serve as the radiation absorbing target and no further addition of carbon was required. Due to the high temperatures involved and the difficulty in heating a gas to those temperatures (by convection from reactor walls), the carbon particles are the key to this process.

Although the technical feasibility was conclusively demonstrated, the use of electricity to provide the high temperatures required doomed it economically. Highly concentrated sunlight can be used to generate the high temperatures needed and provides an environmentally clean option for the production of hydrogen.

The goal of this work is to demonstrate the technical feasibility of this reaction using highly concentrated sunlight as the energy source and to identify the specific technical issues that need to be solved to move the concept forward.

Task 1: Solar Reactor Design

The primary objective of this task will be to modify an existing experimental apparatus (located at NREL) for this work. Two reactor design options will be designed and built. One is based on the injection of a cloud of carbon particles in methane into a quartz reactor tube with the particles directly illuminated by the concentrated sunlight. The other is based on using an intermediate graphite tube to absorb the sunlight and reradiate it to the carbon/methane mixture. In addition, the optics of the existing apparatus will need to be modified for the flux and temperature requirements of this process. A new secondary concentrator will be designed and fabricated for this purpose.

Thermal Dissociation of Methane Using a Solar-Coupled Aerosol Flow Reactor
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Solar Reactor Design						
Complete modifications and installation of reactor system			◆			
Design Evaluation and Cost Analysis						
Complete definition of system components & configurations			◆			

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Task 2: Design Evaluation and Cost Analysis

Based on a preliminary system and component description, a preliminary cost analysis will be conducted to determine the economic potential of this concept. This task will be conducted in partnership with a chemical engineering consultant.

Separation Membrane Development - Savannah River Technology Center

Refineries are the largest consumers of hydrogen. Currently the hydrogen gas is supplied by external sources. Plenty of low partial pressure hydrogen streams exist in the refinery operation. Recovery of hydrogen from the low partial pressure streams to achieve high purity, high-pressure hydrogen is very costly in current technology.

At the Savannah River Technology Center, a new class of composite materials has been developed. The new material contains metal hydride particles surrounded by a porous glass matrix, which allows hydrogen to easily enter the composite and absorb reversibly on the metal hydrides. In a similar process, a composite membrane can be fabricated by coating a thin layer of dense glass matrix by the sol-gel process. The membrane can filter the hydrogen gas from all other gases including poisonous gases. This glass matrix can serve as a screen to prevent other gases passing through and be an excellent hydrogen filter. This filter unit can be used in a methane reformer, water/gas shift reactor, or partial oxidation reactor to pump hydrogen continuously from the reactor to achieve very high yield.

Currently, a feasibility study is being performed to determine the optimum conditions for using sol-gel process to form a glass matrix, which can selectively filter the hydrogen gas. A filter system is being developed by means of a glass matrix coating on a metal or ceramic. The effectiveness of the glass matrix membrane depends on the pore size distribution that can be controlled by the gelating conditions of sol-gel process. The objective is to determine the conditions to achieve the right pore size distribution in the membrane to maximize the selective permeation of hydrogen. Workable filter units will be produced and tested for separation and recovery of hydrogen from the gas mixtures. Performance will be evaluated.

Task 3: Filter Fabrication

Test will be continued to adjust the filter coating conditions and substrate selection for mechanically stable filter.

Task 4: Optimum Filter Fabrication

Based on the data obtained from the previous tasks, an efficient filter will be fabricated. Low cost processes will be determined for filter-production.

Separation Membrane Development
Savannah River Technology Center

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Filter Fabrication						
Create defect free coating		◆				
Manufacture large filter				◆		
Test Reactor						
Construct reactor				◆		
Test reactor					◆	

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Task 6: Membrane Reactor Tests

The performance of the reactor will be evaluated.

Production of H_2 by Superadiabatic Decomposition of Hydrogen Sulfide – Institute of Gas Technology

Since the economics and environmental benefits are favorable compared to existing sulfur recovery processes, the feasibility of the SAC/hydrogen sulfide decomposition approach for hydrogen production must be examined from a technical perspective. The technical objectives for development, demonstration, and commercialization of the process include development of a practical SAC reactor design concept; determination of the optimum reactor operating conditions for decomposition of hydrogen sulfide to hydrogen and sulfur; and selection of a practical gas separation system to produce high purity hydrogen at useful pressures while maintaining high sulfur recovery efficiency.

A number of technical challenges must be met in order to achieve these objectives. Principal among these are defining the thermochemical and kinetic behavior of the hydrogen sulfide decomposition reaction under SAC conditions including back reaction of the decomposition products to hydrogen sulfide; defining the effect of operating pressure on throughput, combustion wave temperature, decomposition conversion, and combustion wave stability; defining the effects of acid gas H_2S concentration and enriched-air oxygen concentration on throughput, combustion wave temperature, conversion, and combustion wave stability; determining the effect of acid gas contaminants on products formed, particularly COS and CS_2 formation from side reaction of sulfur with carbon species in the inlet gas; specification of the SAC reactor including operating mode (switching or continuous), porous media characteristics, operating pressure, gas velocities, temperature profile, gas quenching requirements, and control requirements; scale up the reactor to commercial operation while maintaining combustion wave stability; and selection of practical gas separation devices and H_2S recycle schemes to insure high conversion and recovery efficiencies, with hydrogen delivery at a useful pressure.
A phased developmental approach will be utilized to achieve the process development objectives, with periodic evaluation by the development team members and sponsors to guide subsequent development efforts. The development team will include industrial suppliers/users of sulfur recovery technology and potential hydrogen end users. The SAC reactor analysis will be guided by detail thermochemical and

Production of H_2 by Superadiabatic Decomposition of Hydrogen Sulfide
Institute of Gas Technology

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Reactor Modeling						
Complete detailed modeling plan and cost estimate		◆				
Market and Economic Study						
Conduct market and economic study		◆				
Process Design Definition						
Conduct the process design study and reactor modeling		◆				
Phase II Development Plan						
Complete phase II development plan			◆			
Lab-Scale Testing System Design						
Complete system design			◆			

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kinetic modeling using H_2S-rich fuel gas and air/enriched air feeds. Reactor modeling results will for the basis for reactor development and model verification testing using a full enclosed, lab-scale reactor systems with online gas sampling and analysis capabilities and a sulfur recovery subsystem. This will be followed by overall system analysis design considering air/enriched air feed, heat recovery, sulfur condensation, gas separation, and H_2S recycle requirements based on the modeling and testing results. The system analysis will employ process simulation studies guided by input from industrial suppliers and end users to insure a practical and marketable result. These results will be used to develop a preliminary system design and cost estimate for use in finding commercialization partners and a host site for bench-scale demonstration testing.

Task 1: Reactor Modeling

A numerical model of rich and ultra-rich filtration combustion (FC) of H_2S/air mixtures over a range of equivalence rations, flow rates, and packed bed parameters will be developed. Particular consideration will be given to the hydrogen production via ultra-rich superadiabatic combustion of H_2S where the overall process could be characterized as combustion-based fuel modification. Numerical studies will be conducted to define the structure and properties of FC waves including reaction and chemical product information, develop numerical models for prediction of output hydrogen concentrations in linear and reverse-flow superadiabatic combustors, and optimize the hydrogen production, by-product composition, and energy consumption based on results of numerical simulations. Modeling studies will be conducted based on computational models of filtration combustion waves in a porous media developed for ultra-rich filtration combustion of methane/air mixtures. Standard reaction flux/pathway and gradient sensitivity analysis technique will be applied at each step to identify important reaction pathways.

Task 2: Market and Economic Study

Evaluation of the potential markets will include analysis of both the sulfur recovery markets as well as hydrogen and sulfur end user markets. Factors considered in the analysis will be current and projected hydrogen and sulfur prices, status of competing hydrogen production and combined hydrogen and sulfur recovery processes under development, current size and demand projects for the various hydrogen market sectors including petroleum refining, ammonia, methanol, and fuels, and current size and demand projections for sulfur market sectors, including sulfuric acid, fertilizers, etc. Information on the sulfur recovery, hydrogen and sulfur markets will be used to determine the most favorable potential settings for deployment of the SAC hydrogen sulfide decomposition technology. These settings will be used as the selection criteria to focus selection of the various process design alternatives that must be considered on the most promising applications.

Task 3: Process Design Definition

The project team will develop a preliminary process design for the integrated H_2S to hydrogen and sulfur process. The system will consist of five subsystems: Acid-Gas Preconditioning, SAC reactor, Sulfur Recovery, Gas Separation and Recycle, and Hydrogen Delivery. Several system design variations may be necessary to account for the expected range of acid gas feedstock compositions, process design options, and product and end user market factors. Block flow diagrams of both systems and process flow diagrams of the individual subsystems will be prepared. Mass and energy balances will be developed for each subsystem for the two SAC reactor configurations using acid gas conditions typical of the selected user setting.

Task 4: Phase II Development Plan

Based on the results of the reactor modeling, market and economic, and process design studies, a development plan for Phase II activities will be prepared, including: detailed reactor modeling for one or more reactor configurations; lab-scale testing for model and process design verification; subsystems tests conducted separately or in conjunction with reactor testing, as required; and detailed design and cost estimate for a bench-scale system for field testing at an industrial site. The development plan will provide a detailed parametric test plan for the model verification and process and subsystem testing. Design requirements for the bench-scale field-testing system will also be defined.

Task 5: Lab-Scale Testing System Design

The UIC lab-scale SAC reactor system previously used for the in-house research work conducted jointly by IGT and UIC will be modified to a totally enclosed system to enable flow measurement, sampling and analysis of decomposition reaction products.

Task 6: Reporting

A detailed technical progress report will be completed containing the development plan, cost estimate, schedule, milestones, teaming, and cost sharing information. Two representatives of the development team will attend the May 2000 Peer Review Meeting and will present the Phase I results and Phase II development plan for evaluation by the peer review panel.

Thermocatalytic CO_2 – Free Production of Hydrogen from Hydrocarbon Fuels – Florida Solar Energy Center (FSEC)

The main objective of the research work is to develop a viable process for CO_2-free production of hydrogen by thermocatalytic conversion of different hydrocarbon fuels, e.g. natural gas, propane and gasoline. The process is based on one-step thermocatalytic decomposition (or pyrolysis) of hydrocarbon fuels in the absence of air and/or water. Along with hydrogen, the process also produces pure carbon, currently valuable chemical commodity. This approach eliminates the production of carbon oxides (CO and CO_2) and, consequently, complex and expensive water gas shift reaction and gas separation stages required by the conventional processes of hydrogen production (e.g. steam reforming, partial oxidation and autothermal reforming).

The following issues must be addressed to determine the feasibility of the proposed technology:

- Production of sustainable CO/CO_2-free hydrogen-rich gas mixtures from different hydrocarbon fuels (e.g. methane, propane, gasoline)
- Use of active and stable carbon-based catalysts
- Construction and testing of a bench-scale thermocatalytic reactor for the simultaneous production of hydrogen and carbon

The ultimate objective of the project is the development of an efficient, compact and cost-effective hydrocarbon fuel processor for on-site production of hydrogen-rich gases from natural gas and other hydrocarbon fuels at gas refueling stations. The concept can also be used for CO/CO_2-free production of hydrogen for fuel cell applications.

Task 1: Thermocatalytic Pyrolysis of Hydrocarbons over Carbon-based Catalysts:

Thermocatalytic pyrolysis of methane, propane and liquid hydrocarbons over carbon-based catalysts will be investigated. The catalytic activity of various forms of carbon including, but not limited to, activated carbon of different origin, carbon produced by pyrolysis of polymers and natural organic compounds (e.g. polyacrylonitrile, polymethacrylate, cellulose, etc.) toward decomposition of gaseous hydrocarbons (e.g.

Thermocatalytic CO2 – Free Production of Hydrogen from Hydrocarbon Fuels
Florida Solar Energy Center

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Catalyst Activity, Stability and Deactivation						
Determine effect of carbon deposition		◆				
Study methane decomposition in binary mixtures		◆				
TCR Construction and Testing						
Complete fabrication of a bench-scale TCR		◆				
Test TCR using different hydrocarbon fuels			◆			

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methane and propane) will be examined. The effect of operational parameters (temperature, partial pressure and residence time) on the hydrogen yield for methane and propane pyrolysis over the selected carbon-based catalysts will be examined. The thermocatalytic pyrolysis of liquid hydrocarbons will be studies. The two or three most active carbon-based catalysts will be used to pyrolyze liquid hydrocarbons.

Task 2: Catalyst Activity, Stability and Deactivation:

The effect of carbon source and its surface structure on the catalytic activity and long-term stability toward hydrocarbon pyrolysis and the effect of operational parameters (temperature, residence time) on the carbon catalyst long-term stability and deactivation rate will be studied. The byproducts of hydrocarbon decomposition will be identified and the effect of carbon source and temperature on their yield will be determined. The effect of carbon deposition on the activity of carbon catalysts will also be determined. The transient and steady state decomposition of methane and propane over selected carbon catalysts in the presence of other hydrocarbons (binary mixtures) will be investigated.

Task 3: Thermocatalytic Reactor Construction and Testing:

A bench-scale thermocatalytic reactor will be constructed for hydrogen and carbon production from a variety of hydrocarbon fuels (methane, propane, gasoline).

Sorption Enhanced Reaction Process for Production of Hydrogen (H_2-SER) - Air Products and Chemicals, Inc. (APCI)

Air Products is actively developing an innovative concept -- Sorption Enhanced Reaction (H_2-SER) -- for the production of hydrogen via steam-methane reforming (SMR). The H_2-SER process has the potential to significantly lower the operating temperature of a steam-methane reformer while maintaining high reactant conversion. Thus, this new process offers the possibility of changing the basic concept and engineering design of SMR-based hydrogen production systems, and markedly reducing their cost. Such systems could meaningfully contribute to an acceleration of interest in near- and mid-term energy applications for hydrogen, particularly in the transportation sector.

The concept of SER is based on the reduction of the CO_2 concentration in the reaction zone of the reforming reactor by using an adsorbent material that selectively and reversibly binds carbon dioxide. A process based on this concept would be operated using two or more reactors, and each reactor would be subjected to alternating reaction/adsorption and regeneration steps. By removing CO_2 from the reaction zone, the equilibrium-controlled steam-methane reforming reaction is driven towards high methane conversion even at relatively low temperatures (e.g., 350-550^{o}C). The removal of CO_2 also favors conversion of the water-gas shift reaction, yielding very low CO levels in the reactor effluent stream.

A DOE/Air Products cooperative agreement was implemented in FY95 to promote the development and evaluation of this new process technology. The development plan consists of the following three phases; Phase I: Concept Feasibility, Phase II: Engineering Development, and Phase III: PDU Demonstration.

The major goals for Phase III are to demonstrate and evaluate the feasibility of the fully cyclic H2-SER process in the new process test unit (years 1 and 2), design and build a process demonstration unit, or PDU (year 2 and 3), and operate and evaluate the performance of the PDU (year 3). Plans will also be developed for the application and commercialization of the process. Parallel efforts will be focused on

Sorption Enhanced Reaction Process for Production of Hydrogen (H_2-SER)
Air Products and Chemicals, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Operate Cyclic Process Test Unit						
Demonstrate cyclic steady-state H2 production	◆					
Evaluate sensitivity of process performance			◆			
Revise the process design from PHase II			◆			
Evaluate the economics of the new design				◆		
Scale-Up Production of CO2 Adsorbent for PDU						
Transfer synthesis procedure to vendor for production						
Obtian vendor-prepared adsorbent for SER#2		◆				
Obtain vendor-prepared adsorbent for PDU						◆
Design, Build and Install a PDU						
Identify location for installation of PDU		◆				
Complete the design of the PDU					◆	
Make go/ no go decision					◆	

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improving the properties of the CO_2 adsorbent and scaling-up production of this material to PDU and commercial scale.

The objective of phase III is to Operate the process test unit (SER#2) built in Phase II to demonstrate the continuous, cyclic steady-state H2-SER process, generate process data for the development of a detailed process design, complete a detailed process and economic analysis, scale-up production of the CO2 adsorbent, and initiate commercial development activities.

Task 1: Operate Cyclic Process Test Unit (SER#2) and Evaluate Process Performance

Subtask 1.1: Demonstrate Cyclic Steady-State Production of Hydrogen with the Cyclic Process Test Unit
An experimental, two-bed (each 20 ft long by 1 inch inside diameter) reactor system constructed in Phase II will be used to carry out the cyclic H_2-SER process steps in continuous mode, i.e., repetitive reaction/adsorption and regeneration steps. External electric blanket heaters will be used to provide energy to the reactors. These experiments will demonstrate the cyclic steady-state production of hydrogen using process parameters defined in the current lab-scale unit (SER#1).

Subtask 1.2: Evaluate the Sensitivity of Process Performance to Various Operating Parameters
Experiments will be conducted with the electrically-heated cyclic SER#2 unit to determine the effect of various operating parameters [reactor temperature and temperature gradient, reaction pressure, feed steam to carbon ratio, feed velocity, purge amount and purge pressure] on process performance. Different process cycles will be evaluated (e.g., with and without pressure equalization steps). System performance will be determined by calculating the conversion of feed methane to product hydrogen, average purity of the hydrogen product, $CO/CO_2/CH_4$ impurity levels in the product, and reactor productivity (moles of hydrogen product/kg solid).

The above data set will be used to help direct future experiments with commercial heating equipment (indirect gas heating (IGH) or heat transfer fluid (HTF)). A decision will be made whether to carry these experiments out with the SER#2 unit (modified to include the respective heat transfer equipment) or include it in the scope of the scheduled process development unit (PDU).

Concurrent with SER#2 efforts, the non-cyclic process test unit, SER#1, will be used to provide data to aid operation of SER#2 and evaluate new catalyst and adsorbent systems.

Subtask 1.3 Revise the Process Design from Phase II Based on New Information Obtained from SER#1 and SER#2
The first-pass H2-SER process designs (HTF and IGH) generated in Phase II will be revised as cyclic steady-state process data become available from SER#2. Process designs for a range of hydrogen production capacities will be generated.

Subtask 1.4: Evaluate the Economics of the New Design for Various Hydrogen Production Rates
Economics of new H2-SER process designs will be evaluated by the APCI HYCO group. This will allow comparison of H_2-SER performance with other hydrogen production technologies and permit verification of process economic viability.

Task 2: Scale-up Production of CO_2 Adsorbent for PDU

Subtask 2.1: Transfer the Synthesis Procedure of he Preferred Adsorbent to a Vendor for Production of Adsorbent for the PDU
Production of fully promoted HTC adsorbent for the SER#2 and PDU will be carried out by a vendor at their site. Currently two vendors have been identified and have prepared preliminary samples. Air Products will continue to work closely with them to ensure that their commercial material performs to its

required specifications (e.g., adsorption capacity, kinetics, stability). APCI expects delivery of 100 lbs of promoted HTC in 1QFY00 for testing in SER#2, and 2000 lbs for the PDU in 1QFY01.

Subtask 2.2: Continue to Develop Second Generation Adsorbents with Improved Adsorption Properties
The goal of these efforts is to improve the physical properties of the CO_2 adsorbent and develop additional second-generation adsorbents (H-series). This work will continue since the economics of the H2-SER process can be even more favorable when an adsorbent with higher CO_2 adsorption capacity or more linear CO_2 adsorption isotherm is used. The long-term stability of the HTC and second-generation materials in cyclic reaction and regeneration environments will also be addressed.

Task 3: Design, Build and Install a Process Development Unit (PDU) Producing 0.1 MM SCFD H_2

Subtask 3.1: Identify Location for Installation of PDU
Air Products has identified a potential location (LaPorte) for the PDU and conducted preliminary discussions with the appropriate APCI personnel. Further effort is needed to work out permitting and logistical issues.

Subtask 3.2: Complete the Design of the PDU
This will be accomplished through the APCI GEG HYCO team. Enough detail needs to be developed by the end of 4QFY00 to form cost basis for DOE GO/NO GO decision.

Subtask 3.3: GO/NO GO Decision Point
A GO/NO GO decision will be made based on technical input from the above tasks to decide whether or not to proceed with scheduled PDU activities. Air Products will prepare and submit to DOE a NEPA Review and Determination (Form GO-EF2) for the proposed PDU installation. DOE will make a NEPA determination based on the information provided and will also make a GO/NO GO decision for the PDU.

Subtask 3.4: PDU Installation
APCI will install the PDU and bring on-stream equipment procurement and construction will begin once DOE approval for PDU has been obtained.

Engineering Development of Ceramic Membrane Reactor Systems for converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels - Air Products and Chemicals Inc.

The objective of this program is to research, develop and demonstrate a novel ceramic membrane reactor system for the low-cost conversion of natural gas to synthesis gas and hydrogen for liquid transportation fuels: the ITM Syngas and ITM H2 processes. Through an eight-year, three-phase program, the technology will be developed and scaled up to obtain the technical, engineering, operating and economic data necessary for the final step to full commercialization of GTL conversion and hydrogen generation technologies

Task 1: ITM Materials and Process R&D

Air Products will study engineering fundamentals and evaluate materials, ceramic membrane and process concepts at the bench-scale level.

Engineering Development of Ceramic Membrane Reactor Systems for converting Natural Gas to Hydrogen and Synthesis Gas for Liquid Transportation Fuels
Air Products and Chemicals Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Process Engineering and Economics						
Complete preliminary process designs			◆			
Design and engineer nominal 24 MSCFD PDU				◆		
Make decision to proceed			◆			
Materials and Seals Development						
Develop, demonstrate at process conditions			◆			
Demonstrate sub-scale thin membranes				◆		
Test improved ITM materials				◆		
ITM Syngas Reactor Design and Engineering						
Develop ITM membrane and reactor vessel designs			◆			
Design preliminary PDU membrane and reactor vessel				◆		
Fabricate preliminary PDU membrane				◆		
Materials and Seals Development and Evaluation						
Select provisional seal design for the PDU					◆	
Membrane and Module Design and Fabrication						
Develop and specify PDU membrane & module design					◆	
Nominal 24 MSCFD ITM Syngas PDU						
Initiate construction of the PDU				◆		

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Subtask 1.1: Process Engineering and Economics
Air Products, Chevron, Norsk Hydro, and McDermott will develop process designs and economics, with input from ARCO and the University of Alaska. The results will be used to set objectives for the development of ITM Syngas and H2 materials.

Subtask 1.2: Materials and Seals Development
Air Products, Ceramatec, Eltron and Penn State will jointly perform the materials development to achieve the required performance and stability at process conditions. Air Products and Eltron will test the performance of various ITM/catalyst combinations at pressure. Ceramatec will produce powder and samples for the materials development tasks. Air Products and PNNL will develop high-temperature seals. Penn State University will evaluate mechanical properties. The University of Pennsylvania will provide input on materials.

Subtask 1.3: ITM Syngas Reactor Design and Engineering
McDermott, Ceramatec and Air Products will design the membrane and reactor. Ceramatec will develop the membrane fabrication process. Air Products will design and engineer a reactor vessel for a nominal 24 MSCFD Process Development Unit (PDU), which will utilize sub-scale membrane modules.

At the end of Task 1, a selection will be made for further development of the ITM material/catalyst combinations, the membrane seals, and the membrane reactor design. Process economic and performance data will be used to make the decision to proceed with the scale-up under Task 2.

Task 2: Engineering and Development of an ITM Syngas and ITM H2 PDU and SEP

Task 2 (3.5 years) will validate process concepts in two stages of scale-up, and create an engineering, operating and economic database.

Subtask 2.1: Commercial Plant Economic Evaluation
An advanced ITM Syngas and ITM H2 process will be developed. Based on the results of the Task 2, the economics of operation at the commercial plant scale will be evaluated by Air Products, Chevron, McDermott and Norsk Hydro.

Subtask 2.2: Materials and Seals Development and Evaluation
The combined ITM Syngas testing facilities of Air Products and Eltron Research will be utilized to obtain statistical performance and lifetime data under process conditions for the ITM Syngas materials and seals, fabricated by Ceramatec.

Subtask 2.3: ITM Syngas Membrane and Module Design and Fabrication
Air Products, McDermott and Ceramatec will carry out the detailed design of the membrane, modules and manifolding for the ITM Syngas reactor. Ceramatec will scale up the fabrication of the ceramic membrane reactor modules in a Production Development Facility (PDF) to supply the requirements of the SEP.

Subtask 2.4: Nominal 24 MSCFD ITM Syngas PDU
The components of the ITM Syngas and H2 technology will be demonstrated in a laboratory Process Development Unit (PDU). The PDU will operate at up to an equivalent of 24 MSCFD of syngas capacity, and will be used to performance test sub-scale membranes under process operating conditions for the H2 and syngas /GTL applications.

At the end of Task 2, the projected commercial plant economics for ITM Syngas and ITM H2 will be re-evaluated in by Air Products, Chevron, McDermott and Norsk Hydro, based on the results from the PDU and SEP operations. Three commercial-scale applications will be evaluated: hydrogen generation, offshore GTL, and remote North Slope Alaskan GTL.

Novel Catalytic Fuel Reforming – InnovaTek

InnovaTek, Inc. is applying the advantages of microtechnology in the development of catalytic fuel reforming that also incorporates advanced separations technology. Building on its experience from developing a micro-machined ammonia cracker for a PEM fuel cell, InnovaTek will develop a micro-reactor capable of reforming methanol. The specific problem to be addressed is an energy conversion process to provide clean hydrogen from renewable biomass energy sources. The reformer is used to produce hydrogen from methane or methanol produced through thermochemical processing of biomass. This approach to fuel processing provides a revolutionary breakthrough in terms of system size, weight, and dynamic response when compared to more conventional processing carried out in standard packed bed reactors.

The project will accomplish two primary objectives: thermal and chemical systems analysis and design, and reactor design and fabrication assessment.

Task 1: Thermal Systems Design and Analysis

A one dimensional system model for the reformer will be developed. The model will include the fuel storage vessel and pressurization system, the catalytic reactor, and the heat exchanger. The end deliverable will be a system simulator capable of optimizing the design subject to a variety of constraints and tested against a prototype and against full two/three dimensional predictions.

Task 2: Chemical Systems Design and Analysis

Alternate catalytic materials and structures will be prepared for testing in reforming and oxidation reactions. Catalyst powders will be prepared for incorporation in the reactor. Specific tests will be conducted on both the catalytic systems and the candidate hydrogen separation membranes to determine their physical robustness, their thermal cycling durability and their predicted operational performance. A

Novel Catalytic Fuel Reforming
InnovaTek

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Thermal Systems Design and Analysis						
Complete systems design and analysis				◆		
Chemical Systems Design and Analysis						
Complete chemical systems design and analysis				◆		
Membrane Testing and Analysis						
Complete membrane testing and analysis		◆				
Reactor Design and Integration						
Complete reactor design and integration					◆	
Fabrication Evaluation						
Evaluate fabrication					◆	

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testing and analysis subtask will monitor critical parameters during trial operations of a microchannel reactor with integrated catalyst.

Task 3: Membrane Testing and Analysis

This task will evaluate hydrogen separation membrane technology for purifying reactor output. The critical parameters during trial operations of a microchannel reactor with integrated H_2 separation membrane will be monitored. The components of each chemical stream will be analytically determined using gas chromatography. Digital storage and computational analysis of recorded data will provide the necessary tool for analysis and correlation of test results. Subsequent test runs with adjusted operational parameters will lead to conditions that provide optimum hydrogen purification consistent with efficient fuel consumption.

Task 4: Reactor Design and Integration

Design criteria for the methanol reformer will be established based on the results of Tasks 1-3. Chemical and thermal systems design criteria will be established. Detail designs and design drawings will be created and reviewed.

Task 5: Fabrication Evaluation

This task will evaluate state-of-the-art in micromachining techniques applicable to high temperature systems. Limitations and tolerances associated with these techniques will guide the design process and the choice of materials. An evaluation of the cost and capabilities of microchannel reactor fabrication technologies will be completed.

BIOMASS-BASED PRODUCTION

Hydrogen Production from High-Moisture Content Biomass in Supercritical Water – University of Hawaii (UH)

Current enthusiasm for the use of hydrogen as an alternative transportation fuel is founded on the expectation that the hydrogen will be produced from renewable resources at a competitive price. One method of achieving this goal is the steam reforming of biomass:

(1) $C_6H_{10}O_5 + 7\ H_2O \rightarrow 6\ CO_2 + 12\ H_2$.

In this idealized, stoichiometric equation, cellulose (represented as $C_6H_{10}O_5$) reacts with water to produce hydrogen and carbon dioxide, mimicking the commercial manufacture of hydrogen from methane by catalytic steam reforming chemistry. More realistically, a practical technology must convert the cellulose, hemicellulose, lignin, protein, and extractive components of the biomass feedstock to a gas rich in hydrogen and carbon dioxide, but also including some methane and carbon monoxide. Unfortunately, biomass does not react directly with steam to produce the desired products. Instead, significant amounts of tar and char are formed, and the gas contains higher hydrocarbons in addition to the desired light gases. The total steam reforming of biomass, as envisioned by equation (1) above, remains an elusive goal. UH showed that various charcoals and activated carbons effectively catalyze the steam reforming of many organic compounds in supercritical water and applied for U.S. and foreign patents on this application of carbon catalysts

UH's long term goal is to demonstrate hydrogen production by the total, catalytic, supercritical steam reforming of wet biomass in a commercial prototype reactor. The immediate goals are: (i) to design, and fabricate a commercial prototype reactor with a feed rate of 20 to 100 g/min of potato waste; (ii) to run this reactor continuously (with brief shutdowns for ash and coke removal) for 16 hours or more; (iii) to examine the effects of peak temperatures above 750 °C on the reactor's performance; and (iv) to improve heat transfer and heat recovery within the reactor.

Feedstocks included in this research include food processing wastes (potato wastes, spent beer grains), and biomass (wheat residues, wood sawdust, sugar cane bagasse, etc.) in a corn starch gel. Prior work has shown that sewage sludge is unsuitable for gasification in supercritical water.

Hydrogen Production from High-Moisture Content Biomass in Supercritical Water
University of Hawaii

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Design of the 20-100 g/min reactor and ordering of		■				
Fabricate reactor			■			
Demonstrate gasification of 20-100 g/min throughput potato			■			
Operate the reactor for 16 hr or more				■		
Determine disposition and composition of ash				■		
Determine effect of prolonged operation on carbon				■		
Determine disposition of nitrogen in reactor				■		
Identify effects of peak temperature on reactor					■	

FY 2000 Begins October 1, 1999

The focus in this research is the design, performance, and scaleup of all equipment between the entrance of the feed at 25 °C and 27.6 MPa, and the exit of products at 25 °C and 0.1 MPa. Mr. Robert Divilio has completed a design of a gas separation system for hydrogen production (downstream of the reactor). UH hopes that they will also be able to suggest improvements to its methods of pumping potato wastes and other feedstocks into the reactor.

To operate the reactor with peak temperatures in excess of 750 °C UH must enclose the tubular reactor within a pressure vessel that is isolated from the hot reactor by insulation. Air in the pressure vessel will be at the same pressure as the fluid within the reactor; consequently there will be no pressure gradient across the wall of the hot tubular reactor. It will probably be necessary to cool the pressure vessel by enclosing it in a water jacket at 0.1 MPa. Note that this is the standard design approach for high temperature, high pressure reactors.

Task 1: Design and fabricate a reactor that can accommodate feed rates of 20 to 100 g/min of potato waste

The design considerations include the diameter and length of the tubular reactor that are needed to gasify 100 g/min of potato waste feed. In particular, what diameter and length of the entrance annulus is best to achieve rapid heat-up of the feed? What residence time is needed in the isothermal, void, cracking zone? How large a packed bed of catalyst is needed to deliver a clean water effluent? How large a pressure vessel is required to accommodate the reactor? What are the code requirements for the pressure vessel?

The fabrication considerations include the best employment of existing frame, feed, pressure letdown, and gas sampling systems to house and service the new reactor.

Task 2: Operate the reactor continuously for 16 hr or more

UH estimates that about 8 cleanings and restarts will be needed to operate the reactor for 16 hr. During long runs like this, UH can answer the following questions. How much ash and carbon collect in the entrance region of the reactor? What is the composition of the ash? What is the best method for removing ash (and carbon) deposits from the reactor? What is the disposition of nitrogen (derived from protein in the feed) in the reaction products? What changes does the carbon catalyst undergo during prolonged use? What gaseous products are present when the cold effluent of the reactor is collected at pressure in a pressure vessel?

Task 3: Determine the effects of peak temperatures above 750 °C on the reactor's performance

Earlier work has shown that the gas composition is strongly influenced by the peak temperature reached by the feed in the entrance region of the reactor. Very high hydrogen yields are obtained at peak temperatures above 750 °C, but such high temperatures quickly destroy its current generation of reactors. Since the new reactor will have no pressure gradient across its wall, it will enable gasification studies at high temperature. Under these circumstances, UH wishes to revisit questions related to the effects of heatup rate, peak temperature, gas phase cracking time, and WHSV on the performance of the gasifier.

Task 4: Improve the heat transfer and heat recovery within the reactor

This activity will follow the activities listed above. What are heat demands exist in the entrance region (heatup zone) of the reactor where the feed is heated to 700 °C (or more)? How much does the heat transfer coefficient increase as the flow becomes turbulent in the heatup zone of the reactor?

Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming - National Renewable Energy Laboratory

At present, the commercial production of hydrogen is essentially carried out by catalytic steam reforming of hydrocarbons: natural gas and naphtha. These processes generate, as a side product, carbon dioxide in amounts equal to those of combustion operations, thus contributing to the greenhouse effect. Renewable biomass is an attractive alternative to fossil feedstocks for the production of hydrogen because of essentially zero net CO_2 impact. Biomass includes wood and agricultural residues, municipal solid wastes, industrial wastes from biomass processing (such as pulp and paper operations) as well as dedicated herbaceous and short rotation woody crops. These feedstocks could become available regionally via a diversified choice of species and residues characteristic of each region. The challenge is to convert the biomass into hydrogen at a cost similar to that from existing hydrocarbon-based reforming technologies. If successful, this strategy would substantially help the economic development and diversification of rural areas.

Reforming experiments that have been carried out to date in a fluidized bed system with the carbohydrate-derived fraction of pyrolysis oils have shown promising results, although the catalytic reformer has shown a small decrease in performance with time which can be overcome by catalyst regeneration. At present, NREL feels confident that the process can be taken to the next stage of development: scale up and integration of the fluid bed catalytic reformer with a fast pyrolysis reactor operating at a capacity of 20 kg/h of biomass.

NREL is continuing the development of novel vapor filtration technology, which can be applied to any pyrolysis process. In addition, NREL's patented technology for separating the phenolic oil fraction and its subsequent use as phenol substitute in adhesives is close to commercialization. When implemented, the pyrolysis plant will generate significant amounts of materials (carbohydrate-derived liquids) that could be converted to hydrogen by the catalytic steam-reforming process. Also, other biomass-derived liquids such as hemicellulose-rich solutions from steam-aqueous fractionation of biomass, tall oil from pulping processes, or byproducts from bio-diesel production could be used as potential feedstocks for producing hydrogen.

Biomass to Hydrogen via Fast Pyrolysis and Catalytic Steam Reforming
National Renewable Energy Laboratory

		2000				**2001**
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
H2 Production from Alternative Biomass Feedstocks						
Demonstrate feasibility of processses other than pyrolysis				◆		
Optimization of Steam Reforming Process Conditions						
Demonstrate process conditions that meet target					◆	
Scale Up of the Biomass Pyrolysis/ Reforming Process						
Scale up system integration and operation					◆	

FY 2000 Begins October 1, 1999

During the FY 2000 NREL is planning to continue exploratory and optimization tests using the bench-scale fluidized bed reactor system as well as to scale up the reforming process and integrate it with the NREL Thermochemical User's Facility (TCUF) to produce 1-2 kg/hr of hydrogen (10-20 Nm^3/hr). Specific scientific and technological objectives will be addressed in the following tasks:

Task 1: Hydrogen Production from Alternative Biomass Feedstocks

The purpose of this project is the production of hydrogen from biomass by pyrolysis and steam reforming of the pyrolysis oils. The concept can be extended to include available waste streams from alternative biomass processing as potential feedstocks. One of these streams, hemicellulose-rich aqueous solution from biomass fractionation processes was studied in FY99 and appeared to be a good candidate for steam reforming processing (Milestone report, June 1999). There are other liquid byproducts, such as effluents or wastes from existing technologies (tall oil from pulp and paper process, waste glycerin from biodiesel production, trap grease from food processing) that NREL would like to evaluate as feedstocks for producing hydrogen by catalytic steam reforming process. Samples of those materials will be obtained, analyzed, pretreated (if necessary), and then steam reformed using the 2"-diameter fluidized bed reactor. Process conditions will be optimized considering hydrogen yield and catalyst time-on-stream to be the base criteria. Material balances and hydrogen yields obtained will be used for preliminary technoeconomic assessment of the technology, providing hydrogen production prices from those low-value streams.

Task 2: Automation of the Reforming System

Longer duration experiments require an automatic control of the reforming unit. In FY99, NREL operated for >8 hours with 80% stoichiometric yield in the 2" system. In order to operate for longer periods of time, gas mass flow controllers, on-line monitors for the reforming gas composition, alarms, automated power shut down, and several additions to the hardware and software of the OPTO control system are still required. These will be installed to allow for longer-term operation.

Task 3: Optimization of the Steam Reforming Process Conditions

Though commercial catalysts developed for steam reforming of natural gas and petroleum fractions proved very efficient in converting biomass pyrolysis oil fractions to hydrogen, carbonaceous deposits form in the catalyst bed mostly due to the thermal decomposition of the nonvolatile, oligomeric components of bio-oil. This results in decreasing hydrogen yields as a function of the process time and reduces catalyst time-on-stream. The deposits can be removed from the catalyst by steam or carbon dioxide gasification after which the catalyst recovers its activity. The objective of this task will be finding the process conditions where carbon deposits will not be formed or will be rapidly converted to CO and H_2 thus effectively removing any carbon deposition on the catalyst. NREL is planning to use steam-carbon dioxide mixtures to reform bio-oil fractions using the 2"-diameter reactor (CO_2 was previously observed to remove carbon from the catalyst more efficiently than steam). Another important process variable that NREL will optimize is space velocity (amount of feed per unit of catalyst). Given the observed high reactivity of biomass-derived materials the space velocity could be substantially increased. The increase in the space velocity will be achieved by diluting the catalyst with its inert support; the increase in the feed rate would result in higher gas flow rates in the reactor, which could cause the catalyst entrainment.

Task 4: Autothermal Catalytic Reforming of Biomass-Derived Liquids

Steam reforming is a strongly endothermic process that requires substantial amounts of heat supply. In its experiments an external electric heater has been used to maintain the process temperature. In a larger scale unit, heat will have to be supplied by a cheaper source of energy. A possible option is to use the feedstock (bio-oil or its fractions) for this purpose. Probably the most efficient way to do it is by partially oxidizing the feed in the catalytic bed. This will result in reducing hydrogen yield (by approximately 20%) but will provide the energy necessary for reforming. NREL is planning to use mixtures of steam and oxygen (or steam, CO_2, and oxygen) as the reforming agent and study the impact of different concentrations of water and oxygen in the mixture on the process performance.

Task 5: Scale up of the Biomass Pyrolysis/Reforming Process

Subtask 5.1: Adaptation of the 8"-Diameter Fluidized Bed Reactor for Biomass Fast Pyrolysis Process
An existing fluidized (bubbling) bed reactor will replace the currently used vortex reactor, which is more difficult to operate reliably over a longer time. The FBR will be instrumented (addition of two pressure transducers and of data acquisition and control hardware) and connected to the system. The hook up will require modification to the biomass feeder (transfer screw), plumbing, and electrical connections. The costs of this task will be shared with Biomass Power Program.

Subtask 5.2: Design and Commissioning the Fluidized Bed Reformer
This task will include designing and constructing a 10"-diameter fluidized bed reactor. The reactor will be supplied with an internal cyclone, a perforated gas distribution plate, vapor and liquid feed injection systems, and instrumentation for temperature and pressure measurement and control. The reactor will be designed at NREL then fabricated by an off-site contractor. In addition to the reactor, the unit will include an appropriate heating system and a cyclone.

Subtask 5.3: Coupling the Reformer to the Fast Pyrolysis System
The reformer will be instrumented and hooked up to the biomass pyrolysis reactor, the steam generator, and to the vapor condensation train. Operation of the reformer will be controlled by the OPTO control system. The produced gases, once analyzed for material balances and yield calculations will be directed to the thermal oxidizer and destroyed before release to the atmosphere.

Subtask 5.4: Shake Down of the System; Phase 1 of the Operation of the Unit
In the first phase (FY 2000) the reformer will use pyrolysis vapors generated in the upstream reactor as a feedstock to produce hydrogen. The tests will allow NREL to establish operating procedures and will provide preliminary information on the catalyst performance in the larger system.

Task 6: Deployment Feasibility Study

An opportunity to demonstrate the steam reforming technology for hydrogen production in Blakeley, Georgia was identified in FY99. NREL will continue to facilitate the development of a partnership between public and private organizations to produce the information needed for these organizations to make a decision to move to the demonstration phase. NREL has been working with Enviro-Tech Enterprises, Inc. to identify opportunities for the application of renewable technologies in municipalities, which have control of waste material or power generation or distribution facilities.

NREL will assist Enviro-Tech in building the technical team required to demonstrate the pyrolysis, oil fractionation, adhesive formulation and steam reforming processes. Enviro-Tech, supported by an NREL subcontract, will lead the formation of a new company to perform the eventual demonstration. NREL and the technical partners will work with officials in the state of Georgia to document support for the subsequent demonstration phase. This will include assistance in siting the demonstration facility and using the hydrogen in hydrogen/natural gas blends in bus fleets.

Biomass Pyrolysis for Hydrogen Production – Jet Propulsion Laboratory (JPL)

This task is performed in conjunction with NREL in the context of the reforming of fast-pyrolysis oil in the fluidized bed reactor for hydrogen production. The goal is to obtain a predictive model so as to be able to both optimize the operation of the reactor and to predict the results of scale up. Since its validated biomass particle model showed that there is an optimal temperature for pyrolysis allowing the maximum tar collection, and since its previous vortex reactor model also showed that the optimal reactor temperature is obtained by maximizing oil yield and minimizing oil conversion to gas, the addition of reforming reactions add an additional component to its optimization studies as they will compete with the other reactions.

A simplified solution has been obtained for a laminar carrier gas, compressible (necessary for two phase flows with phase change and reactions) form of the two phase flow with constant temperature (carrier and particles) and single particle size, and further for a binary class of particles (sand and biomass).

Task 1: Dynamics and Heat Transfer

Subtask 1.1: Multiclass particles
This aspect is necessary because it has been shown that the shear stress in single size granular flow is approximately five times that in a binary size mixture. Moreover, it has also been shown that for the same mean size, different fluidization regimes and particle pressures are obtained, according to the size distribution.

Subtask 1.2: Heat transfer model
The heat transfer model is crucial to the prediction of biomass pyrolysis in that heat is transferred from the hot sand to the relatively cold biomass through collisions between sand and biomass particles. Since its previous results showed that fast pyrolysis tar (oils) yield is very temperature sensitive and that yield optimization occurs in a very narrow temperature range due to competing reactions, the biomass temperature must be accurately simulated to enable successful predictions.

Task 2: Biomass chemical reactions

The extensively validated kinetics of Miller et al. will be used in the model.

Biomass Pyrolysis for Hydrogen Production
Jet Propulsion Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Dynamics and Heat Transfer						
Complete multiclass particles model and code		◆				
Complete heat transfer model and code			◆			
Biomass Chemical Reactions						
Complete model and code				◆		
Carrier Flow and Particulate Turbulence Model						
Complete model and code					◆	

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For both Tasks 2 and 3, JPL will debug the code, perform simulations and parametric studies, and validate as much as possible the results of the simulations by comparing with data from the literature. The results obtained will be documented in the open literature and presented at conferences.

Task 3: Carrier Flow and Particulate Turbulence Model

The final coding will be that of the turbulence in the carrier and the particulate flows. Second order closure models constitute the highest possible level of closure currently feasible in terms of computational effort. On the other hand, two-equation models represent the minimum acceptable level of closure that specify an internal length scale. All of the models presented in literature for fluidized beds use a k-ε based gas phase turbulence model (or none at all). It has been argued that the precise turbulence model is not very critical in the dense regions of the bed as the particle motion is completely dominated by collisions. In the present application however, it is important to have an accurate prediction of heat transfer processes and hence to have an accurate turbulence model. The gas phase turbulence model is also important in the prediction of the recirculating gas flow pattern in and around the ‘bubbles’ the fluidized bed which in turn may have effects on the thermal and reactive behavior of the bed. The mass transfer related interfacial term will be modeled based upon the insight into the problem as brought by simulations of the simplified situations in Tasks 2 and 3. The code will be thoroughly debugged and tested.

Modeling of the Supercritical Water Pyrolysis Process – Combustion Systems, Inc. (CSI)

CSI has been developing the engineering tools necessary to bring the Supercritical Water Pyrolysis Process, which was developed at the University of Hawaii, to commercial status.

Task 1: Design of a Fuel Preparation System

This task will be to develop a design for a fuel preparation system that will produce a pumpable biomass paste that can be fed to the Supercritical Water Reactor. During this task, CSI will identify the types of equipment that are commercially available for preparing a biomass slurry that contains 20 percent by weight of biomass. Process steps include receiving and storage, size reduction, mixing with water and cornstarch, and pumping the slurry up to reactor pressures. The feasibility of forming pumpable pastes with higher feed concentrations will also be studied. This task is expected to be complete by May 26, 2000.

Task 2: Innovative Reactor Design

In this task, CSI will develop an innovative reactor design for the Supercritical Water Pyrolysis process. Work at the University of Hawaii has shown that char forms at the entrance of their reactor whenever the concentration of biomass in the feed stream approaches 8 wt %. The char forms in a region of the reactor where its heat transfer analysis shows that the temperatures are between 200 and 400 °C. Its modeling work has shown that minimizing the time that the feed spends in this temperature range can reduce the quantity of char. Furthermore, the University of Hawaii's data suggests that rapid heating of the feed stream results in higher yields of hydrogen. The objective of this task will be to develop a new reactor design that substantially increases the heating rate of the wood paste. One way to achieve this design goal is to mix the incoming paste stream with sufficient preheated supercritical water such that the resulting mixture is above the pseudo critical temperature. This task will be completed by August 25, 2000. An annual report for FY 2000 will be delivered by September 29, 2000.

In addition to these two tasks, CSI will continue to collaborate with the University of Hawaii on their test program. CSI will assist them, where necessary, in the design of their test program and in the analysis of their test results.

Modeling of the Supercritical Water Pyrolysis Process
Combustion Systems, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Fuel Preparation System for Biomass Feed						
Complete design of fuel preparation system				◆		
Innovative Reactor Design						
Complete reactor design					◆	

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Table 3.2 Renewable Production		
Goal: Advance emission-free, and renewable-based hydrogen production technologies towards commercial viability, with a target cost of $10-$15/MMBtu.		
Category	**Project**	**Researcher**
Electrolytic Processes	Solar Photocatalytic H_2 Production from Water using a Dual Bed Photosystem	Florida Solar Energy Center
	Photoelectrochemical Based Direct Conversion for Hydrogen Production	National Renewable Energy Laboratory
	High Efficiency Steam Electrolyzer	Lawrence Livermore National Laboratory
	Photoelectrochemical Hydrogen Production	University of Hawaii
Photobiological Processes	Biological H_2 from Fuel Gases and from Water	National Renewable Energy Laboratory
	Bioreactor Development for Biological H_2 Production	National Renewable Energy Laboratory
	Development of an Efficient Algal H_2 – Production System	National Renewable Energy Laboratory
	Hydrogen Production by Photosynthetic Water Splitting	Oak Ridge National Laboratory
	Maximizing Photosynthetic Efficiencies and Hydrogen Production by Microalgal Cultures	University of California, Berkeley
	A Two-Phase Photobiological Algal Hydrogen Production System	National Renewable Energy Laboratory

ELECTROLYTIC PROCESSES

Solar Photocatalytic H_2 Production from Water Using a Dual Bed Photosystem – Florida Solar Energy Center

The project involves the demonstration of the feasibility of photcatalytically decomposing water into its constituent elements using a dual bed, or modular photosystem under solar radiation. The system envisioned is of two modules, each consisting of a shallow, flat, sealed container, in which microscopic photocatalytic particles are immobilized. The photocatalysts will be chosen as to whether they specifically promote H_2 or O_2 evolution in their respective containers. An aqueous solution containing a redox mediator is pumped between the two chambers in order to transfer electron equivalents from one reaction to the other. The photosystem will feature separate evolution of H_2 and O_2; potentially higher utilization of the solar spectrum, since the two light-absorbing modules will be able to use more abundant, lower energy photons; and cheap reagents, photocatalysts and construction materials, plus minimal processing result in a low-cost module.

In previous work, both modules by themselves have been show to work, selectively evolving either H_2 or O_2 while respectively oxidizing or reducing the redox mediator. The key objective now is to demonstration that the two modules can work together, each absorbing visible wavelength light, and generating enough free energy to perform net water decomposition in the steady state. A number of organic and inorganic compounds have been identified that are good absorbers of solar radiation, and that are energetically capable of performing the various photoredox processes. The work described in Phase I will be to assemble an energy-efficient, materials-compatible photocatalyst//mediator//photocatalyst combination that will demonstrate net water spilling.

Solar Photocatalytic H_2 Production from Water Using a Dual Bed Photosystem
Florida Solar Energy Center (FSEC)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Evaluation of Organic Pigments						
Obtain voltammetric data		◆				
Obtain ionization potential data			◆			
Obtain photoconductivity data				◆		
Film Deposition Technology Development						
Select photoconductive polymers		◆				
Complete comparison to sublimed films				◆		
Demonstration of Photocatalytic Water-Splitting						
Construct and test module					◆	
Participation in International Energy Agency						
Attend Fall experts meeting			◆			
Attend Spring experts meeting					◆	

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Task 1: Evaluation of Organic Pigments as Photocatalytic Materials

Work to date has identified the following organic pigments that appear to have desirable characteristics with regard to photocatalytic water splitting: Quinacridone Red, Isoviolanthrone, Dimethoxy Violanthrone, Indanthrone, Pyranthrone, Indigo, Perylene TCDA, bis (p-chlorophenyl) DPP, Indanthrene Yellow GCN, Indanthrene Black BBN, and Indanthrene Gold Orange. The project will verify whether these materials are suitable for photocatalytic oxidative and reductive water splitting.

Task 2: Film Deposition Technology Development

A fundamental aspect of the dual bed system is that the two photocatalysts should be bound to a surface in their respective modules. While this can be accomplished simply by growing crystals from a solution or sublimed under vacuum, a more general approach would be to blend the photoparticles with a polymeric binder and apply it as if it were paint. From a manufacturing viewpoint, this would represent a major breakthrough in the processing costs associated with module manufacture. On the microscopic level, the dual bed system is somewhat dependent on electronic communication between particles, and in future embodiments of the dual bed concept, between photocatalytic lamina. In that case, the photoparticles must be immobilized in such a way that photo-generated charge can travel through the membrane and not just within the light-absorbing microcell. Two possible approaches can be made: increase the weight percent of photocatalyst within the composite membrane to the point where there is substantial interparticle contact; or suspend the photocatalyst within a polymeric binder that itself exhibits facile conduction of injected charge, and match it to the electronic structure of the photocatalyst, so that photo-generated charge can be injected into the polymer binder for transport across the membrane. Photoconductivity for both of these approaches will be investigated and compared to the sublimed or solution-grown crystalline deposits.

Task 3: Demonstration of Photocatalytic Water Splitting

Lists of H_2-evolving and O_2-evolving photocatalysts will be compiled, and the best photocatalyst//redox mediator//photocatalyst combination will be made for demonstration of photcatalytic water splitting.

Task 4: Participation in the International Energy Agency Annex XIV on Photoproduction of Hydrogen

Work will be conducted with the National Institute of Materials and Chemicals Research and the University of Geneva in preparing immobilized, colloidal metal oxide semiconductors using sol-gel methods to evaluate in the context of dual module photocatalytic water splitting and developing cheap, non-noble metal co-catalysts for use in the dual bed photosystem.

Photoelectrochemical Based Direct Conversion Systems for Hydrogen Production - National Renewable Energy Laboratory

One of the major advantages of a direct conversion system is that the area available for electrolysis approximates that of the solar cell. At solar intensities, this current density is 10-20 mA/cm^2, depending on the type of solar collector and its efficiency. At these current densities, the voltage required for electrolysis is much lower, and therefore the corresponding electrolysis efficiency is much higher. At a current density similar to short circuit photocurrent from a solar cell, hydrogen and oxygen generation is achieved at an applied voltage of approximately 1.35 V, giving rise to an electrolysis efficiency of 91%. Coupling this to a 12% efficient PV array leads to an overall solar-to-hydrogen efficiency of 10.9%. This then is one of the advantages of a direct conversion hydrogen generation system, not only does it eliminate most of the costs of the electrolyzer, but it also has the possibility of increasing the overall efficiency of the process.

An illuminated semiconductor immersed in aqueous solution - a photoelectrochemical (PEC) system - exemplifies such a direct conversion system. These photoelectrochemical systems have been a focus of a number of researchers for over 20 years. For a single gap semiconductor based direct conversion water splitting system, the fundamental requirement of at least 1.4 V implies a minimum bandgap of 1.8 electron volts. An additional requirement is that the semiconductor band edges span both redox potentials of the hydrogen and oxygen evolution reactions. Part of this project is directed at identifying new semiconductors with suitable properties for PEC water splitting, and determining proper surface treatments to enhance reaction rates, and stabilize the surface.

More advanced technologies for PEC water splitting include photovoltaic tandem cells. This technology connects two photovoltaic layers (p-n junctions) with different semiconductor bandgaps in series, one behind the other in a single monolithic device. This arrangement provides the highest theoretical conversion efficiency of any photoconversion system. The combination of lower cost and high efficiency represents an important area of research. Part of this project is directed at designing and optimizing tandem cell technology and integrating it into a photoelectrolysis system.

The goal of this research is to develop a stable, cost effective, photoelectrochemical based system that splits water upon illumination, producing hydrogen and oxygen directly, using sunlight as the only energy input. Theoretical efficiency for tandem junction systems is 42%; practical III-V systems could achieve 18-24% efficiency. Low cost multi-junction amorphous silicon systems could achieve 7-12% efficiency.

Photoelectrochemical Based Direct Conversion Systems for Hydrogen Production
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
High Efficiency Tandem Cell Characterization						
Report on metal ions as catalysts for p-type GaInP2				◆		
Report on viability of nitrides as PEC water-splitting devices					◆	
Low Cost Amorphous Silicon Multijunctions						
Achieve 5% water splitting efficiency					◆	

FY 2000 Begins October 1, 1999

The study of PEC direct conversion systems involves two areas of research: semiconducting materials, and surface treatments. Semiconducting materials can be divided into two types based on their solid state structure: single photon absorbers and multi-photon (multi-junction) devices. Surface treatments involve coatings to address energetic stability under illumination, catalysts for the water splitting reactions and corrosion problems. Its work on semiconductors is primarily focused on multiple photon devices. For surface treatments, NREL's focus is on stabilizing the interface both energetically, and against corrosion.

For multi-junction systems, NREL is studying III-V semiconducting materials (materials are made with various combinations of gallium, indium, arsenic nitrogen and phosphorous); and amorphous silicon based systems. The III-V tandem cell structures are the semiconductors that solid state research groups are focusing on as the next generation of high efficiency (>25%) solar cells. The amorphous silicon (a-Si) systems represent a low cost (albeit lower efficiency) silicon-based direct conversion system.

Its work has shown that the $GaInP_2/GaAs$ system will split water at efficiencies greater than 12%, and it is relatively stable in an aqueous environment. The lifetime of these cells has been extended to 3 days. The a-Si/a-SiC system has also shown promise as a water splitting system. Aspects of this work have generated industrial interest.

Task 1: High Efficiency Tandem Cell Characterization

The primary objective of this task is to increase the stability and efficiency of tandem cell designs. A secondary objective is to identify new materials and study this for efficiency and stability potential. NREL has achieved direct water electrolysis with a novel integrated monolithic photoelectrochemical-photovoltaic design. This photoelectrochemical cell, voltage biased with an integrated photovoltaic device, splits water directly upon illumination; light is the only energy input. The hydrogen production efficiency for this system based on the short-circuit current and the lower heating value of hydrogen is 12.4%. Thus far NREL has not been able to stabilize this system much beyond 3 days of operation, but because of its high efficiency, efforts will continue to identify and understand the factors that limit the efficiency of this design. Research will also continue on the corrosion mechanisms and possible passivating techniques.

As part of NREL's search for semiconductor materials with inherently greater stability, NREL has initiated a study of nitride materials. It is known that GaN is chemically very stable, so much so that device fabricators have not been able to develop a suitable wet chemical etchant for it. It is also known that the composition of $In_xGa_{1-x}N$ can be adjusted to produce a band gap suitable for solar applications.

Identification of solution compositions and additives that stabilize the semiconductor/electrolyte interface will be critical if a more stable PEC-based, water-splitting system is to be developed. The present study is focused on the stability of the p-$GaInP_2$ electrode in aqueous electrolytes of different pHs. Of particular interest is the electrochemical behavior of the illuminated electrode under both open-circuit conditions and cathodic polarization. Investigation of the high efficiency $GaInP_2/GaAs$ system will focus on determining passivating conditions to further reduce or even eliminate corrosion. Further experiments are planned to look at surface pretreatments to see if NREL can increase the lifetime of the catalytic coat.

Task 2: Low Cost Amorphous Silicon Multijunctions

For this work NREL is partnering with Energy Conversion Devices to grow samples specifically for water splitting. For these samples, two areas of research are of interest to us: 1) a device structure that pushes electrons toward the semiconductor/electrolyte interface and 2) protective coatings for the surface that offer minimum light absorption, but stability at high and low pH. The reason NREL want electrons to be driven toward the semiconductor electrolyte interface is because NREL wants hydrogen to be evolved from the illuminated surface. Of the two reactions involved in water splitting (hydrogen evolution and oxygen evolution), hydrogen evolution is the easiest, requiring the least amount of catalyst and it has the lowest overvoltage. NREL also expects that it will be easier to protect a surface under reducing conditions than under oxidizing conditions.

Among the coating of interest are a-SiC, ITO, TiO_2 and SnO:F. Preliminary work at NREL has shown that a-SiC can provide a stable surface layer and is effective at protecting the underlying photovoltaic layers. ITO (indium tin oxide) is also a strong possibility due to its use as a transparent electrode. SnO:F is very stable, but it requires a fairly high substrate temperature for deposition. These higher temperatures can lead to major degradation in a-Si devices.

Task 3: System Design

NREL will continue to develop designs for working PEC water splitting systems that can be studied by the Process Analysis Group. The best multijunction design/ catalytic system will be determined, and NREL will study both high efficiency and low cost systems.

High Efficiency Steam Electrolyzer – Lawrence Livermore National Laboratory (LLNL)

Currently, most of the world's total hydrogen demand is met by hydrogen production from fossil fuels, i.e., by steam reforming of natural gas and by coal gasification. However, hydrogen production from water electrolysis is conceptually much simpler and has no direct adverse environmental impact (emission of greenhouse gases). However, electrolytic decomposition of water for hydrogen production has had no significant commercial impact because the process requires high consumption of electricity, which translates into high production cost. Indeed, an analysis of the (now abandoned) German HOT ELLY steam electrolyzer showed that electricity consumption represented 80% of the overall hydrogen production cost. Therefore, it is obvious that if water electrolysis is to become competitive, electricity consumption must be reduced.

Natural gas is used to (effectively) replace part of the electricity required for the splitting of water. In previous steam electrolyzers, the gas supplied to the cathode side is usually a mixture of steam and hydrogen, while the gas supplied to the anode side is usually air. At zero current, the system has an open circuit voltage of about 0.9 V, depending on the hydrogen/steam ratio and operating temperature. In order to electrolyze water, a voltage that opposes and is higher than the open circuit voltage must be applied to pump oxygen from the steam side to the airside. Clearly, much of the electricity used, 60 to 70% of the total electrical power, is wasted in forcing the electrolyzer to operate against the high chemical potential gradient for oxygen. If a reducing gas, such as natural gas, is used on the anode side to replace air, the chemical potential gradient across the electrolyzer can be reduced and the open circuit voltage can be reduced to zero or even made to reverse in sign. Because natural gas is about one quarter the cost of electricity, replacing one unit of energy of electricity by one equivalent unit of natural gas results in significant cost reduction. On the anode side, the reaction between natural gas and oxygen can be either total combustion or a partial oxidation, depending upon the catalyst used. In the first case, the role of natural gas is just to substitute for electricity. In the second case, a mixture of hydrogen and carbon

High Efficiency Steam Electrolyzer
Lawrence Livermore National Laboratory (LLNL)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Long Term Stability of Catalysts						
Test different catalysts for long term stability		◆				
Large Area Thin Film Deposition Equipment						
Build large area thin film deposition equipment			◆			
100 W Stack						
Design 100 W stack			◆			
Stack Fabrication Process						
Determine stack fabrication process					◆	
Build 100 W stack					◆	
100 W Stack Evaluation						
Evaluate 100 W stack					◆	

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monoxide is formed from the partial oxidation of natural gas. If the carbon monoxide is subsequently water-shifted, the total amount of hydrogen produced in this system will be four times greater than that produced in conventional systems for the same amount of electricity used. Overall, the efficiency (versus primary energy) is estimated to be from 60% to 90% depending on the adopted option. Conventional electrolyzers typically achieve 40% at best.
LLNL will build a 100 W stack during FY 2000.

Task 1: Test the long-term stability of the different catalysts

The water splitting catalyst and the partial oxidation catalyst developed during FY 1999 will be evaluated for long term stability under electrolysis conditions.

Task 2: Build large area thin film deposition equipment

LLNL will scale up the low-cost, thin film colloidal deposition technique for larger area depositions for the manufacturing of large electrolyzer stacks. The potential for processing areas up to 100 square cm will be demonstrated.

Task 3: Design a 100 W stack

As for solid oxide fuel cells, there are two possible stack configurations and operating modes for the electrolyzer, e.g. planar vs. the tubular designs. Various engineering calculations will be done in order to compare and to choose the most optimal design configuration.

Task 4: Determine the Stack Fabrication Process and Build a 100 W Stack

After choosing the stack design, LLNL will develop the different steps in the stack fabrication process. For the tubular design, which is the most likely stack configuration for now, the cathode tube will be made by extrusion. This cathode will serve as support for the thin film electrolyte that electrically connect the single cells together, and the anode will be subsequently deposited using the same technique as for the electrolyte. Much of the processing techniques will benefit from the well developed fuel cell fabrication technology.

Task 5: Evaluate the 100 W stack

Stack efficiency, long term stability and cost will be evaluated for this first electrolyzer prototype.

Photoelectrochemical Hydrogen Production - University of Hawaii

One of the goals of the US Department of Energy's Hydrogen Program is development of high efficiency photoelectrochemical systems to produce hydrogen directly from water using sunlight as the energy source. To meet these goals, a system must be low cost, operate at solar-to-chemical conversion efficiencies greater than 10%, and have long operating lifetimes.

In the early 1990's, the University of Hawaii conducted a systematic comparison of single and multiphoton photoelectrochemical systems which showed that series-connected multijunction (MJ) devices optimized for direct water splitting yielded significantly higher efficiencies than conventional single junction (single photon) systems. The multijunction approach also eliminates the need for direct contact between the semiconductor and electrolyte allowing the use of protective films to prevent corrosion, the primary cause of photoelectrode failure.

Past efforts were focused on developing the critical materials required for photoelectrochemical hydrogen production, such as thin film oxygen and hydrogen evolution catalysts and materials to protect the underlying semiconductor photoelectrode. Research also attempted demonstration of a prototype reactor. Significant progress was made in all these areas. The University of Hawaii developed thin-film catalysts with low overpotentials for both hydrogen and oxygen evolution reactions (CoMo and Fe, and NiOx, respectively). These catalysts exhibited excellent chemical stability with no degradation in performance during more than three years of operation in KOH. Wide band gap amorphous silicon carbide and indium-tin-oxide exhibiting excellent corrosion resistance in KOH electrolyte have also been developed. Solar-to-hydrogen conversion efficiencies of 7.8% in outdoor testing (based on the LHV of hydrogen) were achieved using photocathodes fabricated from triple junction amorphous silicon solar cells.

More recently, the University of Hawaii completed a three-year stability study of thin-film sputter deposited hydrogen and oxygen evolution catalysts in fiscal year 1999. The team developed corrosion resistant ITO and TiO_2 exhibiting optical transparency and electrical conductivity suitable for use as a top contact for photoelectrodes and as an encapsulant for photoelectrodes respectively. A small-scale prototype reactor was fabricated for parallel testing of up to six 1" photoelectrodes. A multi-source thermal evaporation system was installed for depositing CIS solar cells. The researchers also designed a new fully integrated and encapsulated

Photoelectrochemical Hydrogen Production
University of Hawaii

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Photoelectrode/Photoreactor Development						
Test prototypes of planar photoelectrodes		◆				
Test planar a-Si:H photoelectrodes in photoreactor				◆		
Report optimal fabrication process for photoelectrodes					◆	
CIS Material Evaluation						
Complete preliminary survey of corroision characteristics			◆			
Complete literature survey of a-Si, CIS, and catalyst films				◆		
Complete characterization of CIGS films					◆	
Advanced Materials Research						
Fabricate and test ITO/TIO2 bilayers		◆				

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photoelectrode structure that eliminates the need for transparent catalysts. The conceptual designs were also modified for a low-cost photoelectrochemical reactor.

At the Hydrogen Program Review in May 1999, a new photoelectrode design allowing use of planar, series connected solar cells, was described. This new photoelectrode design opens the door to use of higher efficiency semiconductor materials not previously considered for solar hydrogen production. The use of materials, such as copper-indium-diselenide cells with reported solar efficiencies exceeding 18%, offer the possibility for photoelectrochemical cells operating at almost 15% efficiency. The objective for FY2000 is to demonstrate high efficiency, long-life production of hydrogen using the new photoelectrode configuration, initially with amorphous silicon and later with high efficiency copper-indium-gallium-diselenide (CIGS) cells.

Task 1: Photoelectrode/Photoreactor Development

Side-by-side encapsulated photoelectrodes, per the new design, will be constructed. Plans for the proposed effort include development of the process sequence for fabrication of a-Si:H based photoelectrodes. Photoelectrodes will be tested under natural sunlight with gas collection.

Task 2: CIS Material Evaluation

The strong absorption characteristics of CIGS have, to date, precluded development of monolithically stacked multijunction solar cells and its use in photoelectrodes for water splitting. However, the new side-by-side encapsulated design proposed for development allows side-by side series connected cells, opening the door for very high efficiency thin film photoelectrodes. We will evaluate the electrical and corrosion resistance properties of CIS and CIGS films and diodes.

Task 3: Advanced Materials Research

Although significant progress has been made in the development of highly stable hydrogen and oxygen evolution catalyst films, corrosion resistant semiconductors, and protective coatings, re-optimization for use in side-by-side electrodes is required. We will also explore alternative protective films.

Task 4: Engineering Analysis

Under this task, we will utilize our optical and equivalent circuit modeling capabilities to develop quantitative comparisons of the performance characteristics of CIGS and a-Si:H based photoelectrodes. These will be used in conjunction with experimental results on performance and stability to identify the most promising material and configuration for development in subsequent phases of larger area photoelectrodes.

PHOTOBIOLOGICAL PROCESSES

Biological H_2 from Fuel Gases and from Water - National Renewable Energy Laboratory

An economic process for producing H_2, biologically or chemically based, would ideally be H_2O derived, solar driven, highly efficient, durable, insensitive to H_2 partial pressure, and inexpensive to build and operate. Of the biological options, systems of intact cells of photosynthetic bacteria are the most advanced. Unlike cyanobacteria or algae, photosynthetic bacteria do not oxidize H_2O and do not directly fulfill the first criterion. They do, however, evolve H_2 from biomass (previously generated from sunlight, H_2O, and CO_2). These bacteria use several different enzymatic mechanisms with near-term commercial potential for biological H_2 production from biomass. One mechanism in particular looks promising for applications as a biological conditioning agent for upgrading thermally generated fuel gases to a level where they can be directly injected into hydrogen fuel cells. This same system has potential to subsequently evolve into a second generation photobiological method to produce H_2 from H_2O.

The near-term project goal is to investigate and optimize the microbes and conditions that enhance bacterial fuel gas conditioning for H_2 production. A mid-term goal is to create a transgenic cyanobacterial strain containing an O_2-tolerant bacterial hydrogenase that will simultaneously evolve H_2 and O_2 from H_2O.

A unique type of hydrogen-producing activity was found in a strain of photosynthetic bacteria that functioned only in darkness to shift CO (and H_2O) into H_2 (and CO_2). NREL have since isolated more than 400 strains of photosynthetic bacteria from local sites that perform this shift reaction in darkness, and will also quantitatively assimilate CO into new cell mass in light. NREL has tested many of its strains for CO shift activity and growth with crude (water-scrubbed only) fuel gases (primarily CO and H_2) generated from thermally gasified wood chips. In darkness, all of the isolates respond by shifting the CO component of the fuel gas into additional H_2, thereby leaving a product gas highly enriched in H_2 (with CO_2 and trace pyrolysis gases). At ambient temperature and pressure conditions and starting from 20% CO in a gas phase, less than 0.1 ppm of CO remained at equilibrium. The product gas can be fed directly into a phosphoric acid or PEM fuel cell with generation of electrical power. The bacterial culture can be readily grown photosynthetically solely on synthetic fuel gas to generate a high mass culture. It can then be placed in continuous darkness for a year or more with nearly constant shift activity. A small amount of metabolic energy is conserved in darkness, sufficient to maintain enzymatic machinery, perhaps indefinitely. Bacterial rates as high as 3.5 mmol H_2 produced from CO/min g cells were obtained from vigorously agitated cultures at low cell density and a temperature of 30^{o}C.

Biological H_2 from Fuel Gases and from Water
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
H2 from Biomass						
Increase bacterial loading in gas-phasse bioreactors					◆	
H2 from Water						
Characterize bacterial hydrogenase for O2 resistant activity					◆	

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Microbiology research focuses on two different, but related, tasks. The near-term task is designed to characterize the bacterial water-gas shift reaction at biochemical and genetic levels so that it can be further enhanced in both activity and stability of hydrogen production from thermally gasified biomass at PDU-scale levels. The longer-term Task 2 will exploit special evolving hydrogenases from bacteria that have been isolated and bred to be oxygen resistant, and genetically transfer the necessary proteins to a cyanobacterial host where they can function in the simultaneous photogeneration of hydrogen and oxygen from water.

Task 1: H_2 from Biomass

Bacterial water-gas shift rates appear to be under an energy-state control. The rates can be considerably enhanced by chemical uncouplers of ATP synthesis which dissipate membrane potential. This condition is similar to the increase of ethanol synthesis seen in yeast when entering into stationary phase of growth. Carbon and redox balances will be performed under active and inhibited anaerobic CO growth conditions using GC and HPLC analysis of any excreted products. Molar growth yield determinations will be made and compared to those (~10.2 g/mol ATP) obtained for dark, anaerobic respiratory and fermentative conditions. This calculation should be very informative in giving ATP yields per CO shifted as well, and help explain the biochemical mechanism of conserving energy from electron transport reactions occurring at this very low redox potential. There are no other defined examples in biological systems.

A nearly positive selection technique has been developed to isolate mutants affected in water-gas shift and hydrogen uptake reactions based on their conditional sensitivity to photo-oxidative killing conditions. A complete library of such mutants will be generated encompassing all encoded proteins. Constitutively over-expressed, water-gas shift mutants will be sought by examining their revertants.

Gas-phase bioreactors have the capacity to maintain immobilized bacteria at much higher concentrations than aqueous reactors, and there is far less mass transfer limitation. NREL has been binding bacteria to high-surface-area nylon fibers, but electron microscopy indicates that only 10-20% of the fiber surface is coated with bacteria. Manipulation of binding conditions, especially the concentration of divalent cations, should significantly increase bacterial binding and thereby decrease the required bioreactor volume.

Task 2: H_2 from Water

The hydrogenase enzyme that mediates hydrogen production from CO has been selected in a number of bacterial isolates to be relatively insensitive to the inhibitory effects of oxygen. NREL has used genetic variants to further select additional oxygen resistance, and mutated the uptake hydrogenase so that there is less than 1% of its activity remaining that could confuse characterization of the evolving hydrogenase. The evolving hydrogenase has been purified and can now be examined for its oxygen stability without any qualifications about possible contaminant activity. With the aid of M. Heben's mass spectrometer, the purified enzyme will be monitored for activity and durability in hydrogen evolution with various levels of oxygen simultaneously present.

The purified hydrogenase enzyme will be incorporated into liposomes and depleted membrane preparations to determine its capacity to integrate and orient into membranes. In this regard, NREL expects the protein to readily partition into the membrane, much as do membranes with reconstituted reaction centers. Recovery of activity will be used to quantitate successful self-insertion.

Creation of a cyanobacterial hybrid that will produce hydrogen under oxygenic conditions will probably require not only the bacterial hydrogenase but also the electron donor/cofactor to link to endogenous, photo-reduced ferredoxins. The identity of this donor is not known, but should become apparent through biochemical investigation of the library of shift mutants previously described. Completion between different mutant membranes in reconstitution of activity will also be examined. Gene transfer work will be initiated with a cyanobacterial recipient.

Bioreactor Development for Biological H_2 Production - National Renewable Energy Laboratory

A large number of bacterial strains have been isolated which perform the water-gas shift reaction on syngas ($CO+H_2O = H_2+CO_2$). At biological temperatures (<50°C), the equilibrium constant for the shift reaction is in excess of 30,000, ensuring that the biologically catalyzed reaction can readily approach completion with little residual CO. The bacteria can also oxidize H_2S and COS from gas streams. The conditioned product gas is sufficiently clean for direct injection into PEM or PA fuel cells.

The near-term project goals are to develop bioreactors with enhanced mass transfer capabilities that will promote an economic biological conditioning of fuel gases for direct use in fuel cells, and to demonstrate the water-gas shift reaction on syngas produced from steam reforming of natural gas and biomass gasification.

A significant amount of previous work has indicated that mass transfer of gaseous CO into the aqueous phase of the bacteria is the rate-limiting step of the process. Vigorously agitated bacterial cultures at low cell densities are able to shift CO into H_2 at rates up to 3.5 mmol per min per g cells, while less-actively stirred cultures at more normal cell densities (2-6 g cells per liter) exhibit H_2 production rates of 0.01-0.1 mmol per min per g cells. In addition, an increase in shift rates with increased CO pressure was linear up to 13 atm of 10% CO.

Simple, low-energy methods to enhance mass transfer have proven to be partially effective. Bacteria immobilized on the surfaces of hollow fibers have remained constantly active for more than one year with only occasional changes of medium. However, the hollow fiber reactors are relatively expensive. Bacteria were also immobilized on the surfaces of nylon beads or fibers. After draining away the bulk water phase, passage of gaseous CO through the interstitial zone resulted in its effective shift into H_2. Rates of 0.1-0.5 mmol H_2 per min per g cells were estimated over 70 days. Helical bubble-train bioreactors employing suspended bacteria in an aqueous phase exhibited shift rates of up to 0.7 mmol H_2 per min per g cells for shorter periods until build-up of carbonic acid in the liquid medium inhibited the bacteria. Maintaining pH control of the medium by alkali titration extended the active production period, but the increased ionic strength also became inhibitory.

The present focus of the work is on the development of improved bioreactor designs, and on collecting performance data using syngas streams produced by steam reforming and biomass gasification.

Bioreactor Development for Biological H_2 Production
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Bioreactor Design and Scale-Up						
Complete reactor model		◆				
Evaluate reactor internals for CO shift performance					◆	
Conduct mass-balance experiments for SCP production					◆	
Research/ Demonstration Skid						
Demonstrate "real-world" bioreactor					◆	

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Bioreactor development work is divided into two tasks. The first task involves the development of an optimum bioreactor design, while the second task involves work on a research/demonstration skid that combines syngas production with microbial CO shift for syngas cleanup.

Task 1: Bioreactor Design and Scale-Up

In the past year, the mass transfer coefficients for CO transfer for the bioreactors used for the CO-shift reaction have been determined, and appear to be consistent with those reported in the literature, reinforcing its belief that the CO shift reaction is mass-transfer limited. A newly designed laboratory-scale CO-shift bioreactor is currently undergoing testing to demonstrate enhanced CO-shift productivity. The productivity data from these experiments will be used to update the 1996 economic analysis of this process. Three specific issues will be addressed in FY2000.

<u>Subtask 1.1: Reactor Modeling</u>
During the development of the laboratory-scale reactor assembly in FY99, it became clear that a detailed reactor model was required for the analysis of the experimental data. A preliminary version of this model has already been developed, but a more detailed version will be necessary to fully interpret all the data.

<u>Subtask 1.2: Improved Reactor Internals</u>
The newly designed bioreactor uses special reactor internals to enhance gas-liquid mass transfer. While the current reactor design is very promising, it is not clear that this is the best possible design. For example, it should be possible to increase the cell density in the bioreactor, and therefore the volumetric productivity, by using porous internals to promote the development of a stable biofilm within the reactor. NREL will perform experiments to determine the relative efficiency of different reactor internals, including both porous and nonporous materials.

<u>Subtask 1.3: Single-cell Protein Co-product</u>
The photosynthetic bacteria that are used for syngas conditioning can also be used as a source of inexpensive single-cell protein (SCP) for animal feed. The bacteria can metabolize CO under both light and dark conditions, but growth (and therefore SCP production) occurs only in daylight hours. The production of a second product (besides hydrogen) should improve the economics of the process. Before a complete economic analysis of this process enhancement can be performed, the rate of SCP production must be quantified. NREL will perform mass balance experiments to quantify the rate of SCP coproduct production during syngas conditioning.

Task 2: Research/Demonstration Skid

Most work to date on this process has used synthetic CO/H_2 feed streams. In a real-world application, syngas will be supplied to the bioreactor either by reforming a gaseous or liquid hydrocarbon fuel, or by biomass gasification. The syngas produced by either of these processes will contain other species besides CO and H_2. For example, syngas produced by propane reforming will likely contain uncracked propane and other hydrocarbons, while syngas from biomass gasification is known to contain quantities of ash and tar. The ability of the bacterial conditioning system to handle “real” syngas streams has not yet been demonstrated. NREL has developed a computer-controlled research/demonstration skid that consists of a steam generator, a thermal reformer, and associated biological shift reactors. A near-infrared (NIR) CO monitor is used to measure and regulate syngas flow to maintain less than 10 ppm residual CO in the conditioned gas. A 50W PEM fuel cell completes the assembly.

The “real-world” demonstration will proceed in two steps. First, an outdoor bioreactor will be continuously operated on reformer gas at the OPTA site for at least 30 days in order to determine the long-term effects of a relatively clean synthesis gas. Then, a downdraft biomass gasifier with water scrub will be added to the research/demonstration skid. After shakedown and troubleshooting, the gasifier will be used to produce the syngas feed to an outdoor bioreactor at flowrates in excess of 300 cm^3/min.

Development of an Efficient Algal H_2-Production System - National Renewable Energy Laboratory

The concept behind the project is to apply classical and molecular genetic techniques to develop a green alga capable of sustained photobiological H_2 production at high rates in air for use in a direct water-splitting process that can be commercialized for renewable fuel production.

The goal of the project is to generate O_2-tolerant, high H_2-producing mutants from the green alga *Chlamydomonas reinhardtii*, test them in a laboratory-scale system for continuous photoproduction of H_2 under aerobic conditions, and collaborate with other national laboratories and universities in improving the efficiency of algal H_2 production.

Hydrogen production by green algae has significant advantages over other biological systems: ATP production is not required, high theoretical efficiencies are possible, and water is used directly as the source of reductant with no stored intermediary carbon metabolites. Currently, the main practical biological limitations to using green algae for photobiological H_2-production are the sensitivity of the reversible hydrogenase to O_2 and low algal photosynthetic conversion efficiencies at solar light intensities. NREL will address the former problem, by generating and selecting for O_2-tolerant, H_2-producing mutants of *C. reinhardtii* using both classical and molecular genetic approaches.

There is sufficient precedent in the literature to warrant attempts to generate an O_2-tolerant hydrogenase in *C. reinhardtii* at this time. For example, O_2-tolerant hydrogenases have been reported in non-photosynthetic bacteria, photosynthetic bacteria, and *C. reinhardtii* mutants (although mutants in the latter organism were not preserved for future studies). Also, recent studies involving site-directed mutagenesis of the uptake hydrogenase from the bacterium *Azotobacter vinelandii* indicate that a single amino acid change in the sequence of one of the subunits of the enzyme alters the O_2-tolerance of the enzyme. Its classical genetic approach will involve mutagenesis and selection under both photoreducing conditions (which favor the O_2-tolerant, H_2-uptake activity of the enzyme), as well as for survival under H_2-producing conditions (which favor the O_2-tolerant, H_2-evolving activity of the hydrogenase). This will allow NREL to select for mutants that not only show increased O_2 tolerance but may also exhibit decreased levels of the oxy-hydrogen back reaction. In a parallel approach, NREL will attempt to clone the reversible hydrogenase gene in *C. reinhardtii* and use site-directed mutagenesis to specifically target its O_2 tolerance properties.

Two classical mutagenesis/selection approaches and two molecular biological approaches will be used to isolate O_2-tolerant, H_2-producing mutants of *Chlamydomonas reinhardtii*. It is expected that the approaches will yield mutants that contain either an O_2-tolerant hydrogenase, or mutants in which O_2-tolerance to H_2 production is conferred by mutations on other genes. Mutant strains isolated as above will as appropriate be characterized in detail and tested for the continuous production of H_2 under aerobic conditions. Ultimately, NREL will transfer the O_2-tolerance traits to algal mutants also displaying high

Development of an Efficient Algal H_2-Production System
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Generation and Selection of Mutants						
Demonstrate H2-production activity in new algal mutant					◆	

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photosynthetic conversion efficiencies (developed by other groups in this program) in order to produce a "super-strain" that could be tested for commercial viability.

Task 1: Generation and Selection of Mutants

The application of two selective pressures, based either on the H_2-producing or on the H_2-uptake activity of the reversible hydrogenase have been combined with the application of a chemochromic screening technique to isolate H_2-producing mutants of *C. reinhardtii* with increased tolerance to O_2. Many clones with a higher O_2 I_{50} (estimated from the rates of H_2 evolution in the dark, induced by the addition of chemical reductants) were isolated this past year. However, the current O_2 I_{50} assay includes the addition of reduced dithionite to the cell cultures, following inactivation of the hydrogenase by O_2. This may result in re-activation of the hydrogenase and, consequently, in higher apparent enzyme activity following O_2 inactivation. NREL will re-evaluate the assay and confirm the putative higher O_2 tolerance of the isolated clones by other means that do not involve possible reactivation of the hydrogenase. NREL will also increase the stringency of its selective procedures and submit its best clones to further rounds of mutagenesis/selection/screening.

Task 2: Molecular Biological Approach

NREL is pursuing a parallel approach for the isolation of O_2-tolerant mutants involving molecular biological techniques will continue to be developed. The objectives of this approach are twofold: (a) to clone the reversible hydrogenase gene from *C. reinhardtii* in order to give NREL access to site-directed mutagenesis as a means of specifically increasing the O_2 tolerance of the enzyme; and (b) to identify other proteins that may be important for the activity and stability of the hydrogenase under aerobic conditions. In order to clone the algal reversible hydrogenase gene (objective (a) above), NREL will finish the construction of a subtracted expression library of induced minus non-induced genes (which will also be used in identifying other proteins required for optimal H_2 evolution activity, objective (b) above), and RT-PCR amplify mRNA from induced cells using degenerate primers specific for the hydrogenase. Both techniques assume that the hydrogenase is transcriptionally regulated. The clone carrying the hydrogenase gene in (a) will be identified by means of a specific polyclonal antibody (generated last year) against *C. reinhardtii* hydrogenase, or by a DNA probe. Initial results on the RT-PCR approach were discouraging, since the amplification products were identified as DNA coding for proteins other than the hydrogenase. However, recent results using a new plasmid preparation led to the amplification of a DNA sequence that encodes for much of the published N-terminal portion of the reversible hydrogenase. NREL's efforts will focus on trying to isolate the complete gene by probing a cDNA *C. reinhardtii* library constructed at NREL from mRNA extracted from anaerobically induced cells with a DNA probe containing the amplified gene sequence. The identity of the gene will have to be confirmed by analysis of its sequence (by comparison with the sequence of other known hydrogenases) and, perhaps, by heterologous expression of the gene in E. coli. If the preliminary results from the RT-PCR work are negative (suggesting that the published N-terminal sequence of the hydrogenase is not correct), NREL will consider other approaches for obtaining the correct gene (or protein) sequence. These include re-isolating the enzyme according to published procedures, or using chemochromic sensor screening to probe an insertional mutagenesis library (obtained from Prof. Melis, UC Berkeley) for clones that cannot produce hydrogen.

Hydrogen Production by Photosynthetic Water Splitting - Oak Ridge National Laboratory (ORNL)

The objective of this research and development project is the development of a commercially viable method for the production of renewable hydrogen by photosynthetic water splitting. The great potential of hydrogen production by microalgal water splitting is predicated on quantitative measurement of the algae's hydrogen-producing capability, which is based on the following: (1) the photosynthetic unit size of hydrogen production; (2) the turnover time of photosynthetic hydrogen production; (3) thermodynamic efficiencies of conversion of light energy into the Gibbs free energy of molecular hydrogen; (4) photosynthetic hydrogen production from sea water using marine algae; and (5) the potential for using modern methods of molecular biology and genetic engineering to maximize efficiency of hydrogen production.

ORNL's work on the thermodynamic driving pressure of photosynthetic hydrogen production is continuing. Recent data suggest that for both *Chlamydomonas* and *Scenedesmus* the pressure at which hydrogen is evolved is close to thermodynamic equilibrium. In addition, ORNL is conducting collaborative research with the University of California, Berkeley, who is providing long-term steady-state measurements on the concept of a single-organism, two-stage process for hydrogen production in green algae.

Task 1: Oxygen-Tolerant Mutants for Renewable Hydrogen Production

One of the most important goals of renewable hydrogen production by photosynthetic water splitting is the development of oxygen-tolerant hydrogenase-containing algal mutants. The significance of oxygen-tolerant hydrogenase mutants is that the oxygen that is concomitantly evolved during the normal process of light activated hydrogen production from water will not serve to inhibit further hydrogen evolution. *Chlamydomonas* mutant 141F2, isolated at the National Renewable Energy Laboratory (NREL), has promising properties as a first step in this direction. In this task, ORNL will continue collaboration with NREL on the further testing of oxygen-tolerant mutants.

Hydrogen Production by Photosynthetic Water Splitting
Oak Ridge National Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Oxygen Tolerance						
Test mutant 141F2			◆			
Test mutant 104G5				◆		
Linearization						
Test mutant DSP521					◆	
Driving Pressure						
Test Scenedesmus			◆			
Test Chlamydomonas				◆		
Single Org., 2-Stage						
Test with Acetate					◆	
Test without Acetate						◆

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Task 2: Linearization of the Light-Saturation Curve of Photosynthesis

In addition to development of oxygen-tolerant hydrogenases, linearization of the photosynthesis and hydrogen light-saturation curves is a key scientific challenge for the field of renewable hydrogen production by photosynthetic water splitting. Since photosynthesis saturates with increasing light intensity, a loss of efficiency and potential productivity occur at higher solar irradiances. ORNL will continue working with the promising results that have been obtained thus far by testing additional mutants of *Chlamydomonas* that have smaller-than-normal light harvesting antennas. From a practical and economic point of view, the ultimate goal is to develop an algal system that has a completely linear light saturation curve.

Task 3: Thermodynamic Driving Pressure of Photosynthetic Hydrogen Production

In this task hydrogen-evolution from common algae such as *Chlamydomonas*, *Scenedesmus*, and *Chlorella* will be tested for their ability to photo-produce hydrogen against a head pressure of varying partial pressures of hydrogen. Initial results in this area suggested that *Scenedesmus* had a significantly higher driving pressure than *Chlamydomonas*. However, this is not the case. In this task, ORNL will continue its studies hydrogen production in hydrogen atmospheres. Development of an algal system that has a high thermodynamic driving pressure is an important practical goal for DOE's Hydrogen Program since it is an important component of the development of practical photo-biological reactors.

Task 4: Single-Organism, Two-stage Process for Hydrogen Production in Green Algae

Prof. A. Melis, University of California at Berkeley, has proposed the concept of a single-organism, two-stage process for hydrogen production in green algae. The idea is that sulfur deprivation induces loss of oxygen evolving activity. Prof. Melis proposes to take advantage of this property to partially overcome the oxygen sensitivity problem of hydrogenase referred to above. Using its unique assay system for simultaneous measurements of hydrogen and oxygen production and carbon dioxide assimilation, ORNL will work with colleagues at UC Berkeley to further test this concept of hydrogen production.

Maximizing Photosynthetic Efficiencies and Hydrogen Production by Microalgal Cultures - University of California, Berkeley

The goal of this research is to produce genetically engineered microalgae with enhanced photosynthetic productivity and hydrogen production under mass culture conditions. To achieve this, it is necessary to optimize the light-utilization properties of the cells, a solution that requires reduction in the number of the chlorophyll molecules that service the two photosystems. Thus, the goal is to isolate microalgal mutants with a truncated chlorophyll antenna size. This will be achieved through physiological manipulations, DNA insertional mutagenesis/screening and biochemical/molecular analyses of *Chlamydomonas reinhardtii* cells. A truncated light-harvesting chlorophyll antenna size for photosystem-II and photosystem-I will result in a relatively higher light intensity required for the saturation of photosynthesis in individual cells. However, it will permit an overall greater solar energy conversion efficiency and cellular productivity in dense cultures because it will minimize wasteful dissipation of bright incident sunlight and mutual cell shading. A feasibility study was conducted on the question of maximizing solar use efficiency and photosynthetic productivity in green algae by minimizing the chlorophyll light-harvesting antenna size of the photosystems. It was shown that, in mass culture, algal strains which possessed a transiently truncated chlorophyll antenna size exhibit ~3 times greater rates of photosynthesis and hydrogen production than could be achieved with fully pigmented cells. The research seeks to develop green algal strains having a permanently truncated chlorophyll antenna size to be used in photobiological hydrogen production.

Sustained photobiological hydrogen production has been achieved in the laboratory via a single-organism, two-stage process with the green alga *Chlamydomonas reinhardtii.* This novel approach features a temporal separation of oxygen evolution and hydrogen production in the light, based on the metabolic regulation of photosystem-II function in the green alga *Chlamydomonas reinhardtii.* Thus, Stage 1 in this process generates O_2 and metabolites by photosynthesis to energetically enrich the cells. Stage 2 photoproduces H_2 with a concomitant consumption of cellular metabolites. No O_2 evolution takes place in Stage 2. The two stages can be made to alternate through the use of a newly discovered metabolic switch (US patent application pending), thereby ensuring the operation of the Stage 1-Stage 2 cycle *ad infinitum.* The simple and straightforward approach of the two-stage process has thus resulted, for the first time in the 60-year history of this field, in the photoproduction of significant amounts of H_2 gas in the laboratory. The research seeks to improve the yield of this novel Single-Organism, Two-Stage Biophotolysis and Hydrogen Production method.

Maximizing Photosynthetic Efficiencies and Hydrogen Production by Microalgal Cultures
University of California, Berkeley

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Truncated Chlorophyll Antenna Size of Photosystems						
Expand DNA insertional mutagenesis library			◆			
Complete cyropreservation of the DNA insertional library				◆		
Complete solar conversion efficiency measurements		◆				
Complete southern blot analysis of transformants			◆			
Single-Organism, Two-Stage Biophotolysis						
Test various approaches to improve H2 production					◆	
Investigate halotolerant green alga in H2 production				◆		
Investigate BioHydrogen genomics/informatics					◆	

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Task 1: Truncated Chlorophyll Antenna Size of the Photosystems

Subtask 1.1: DNA Insertional Mutagenesis Library
UC Berkeley will expand the library of *Chlamydomonas reinhardtii* DNA insertional transformants from the current 6,500 to 10,000 total and make provisions to share the additional transformant with NREL.

Subtask 1.2: Cryopreservation
UC Berkeley will continue with the development and testing of the cryopreservation method that will permit the indefinite storage of the above library. This library will be a significant resource for the DOE H_2 program.

Subtask 1.3: Solar Conversion Efficiency Measurements
UC Berkeley will characterize the structural-functional organization and measure the solar conversion efficiency of the photosynthetic apparatus in selected *Chlamydomonas reinhardtii* transformants (currently at hand), which have a truncated chlorophyll antenna size. Publish the work in respected peer-reviewed journals.

Subtask 1.4: Genetic Analysis of Truncated Chlorophyll Antenna Mutants
Genetic crosses of the selected transformants will test for co-segregation of the "truncated antenna" and "arg+" phenotypes in the mutants. Linkage of the "truncated antenna" property to the arg+ gene insertion will be tested by analysis of the progeny from the back-cross of the putative "truncated antenna" strains with the arg-2 auxotrophs. Mutants will be selected on the basis of co-segregation of the "truncated antenna" and "arg+" phenotypes. This co-segregation is an important prerequisite for the subsequent cloning of the gene interrupted by the exogenous DNA insertion because it signals the presence of the "tag" in the position of the lesion.

Identification, cloning and sequencing of the gene(s) responsible for the down-regulation of the Chl antenna size in Chlamydomonas reinhardtii will open the way for direct manipulation of the Chl antenna size in many other algae and higher plants of interest to the DOE Hydrogen Program.

Subtask 1.5: Southern (Genomic) Blot Analysis of Transformants:
Genomic DNA of cells transformed with the cloned DNA will be subjected to Southern blot analysis with a probe specific for the *ARG7* gene and, separately, with the cloning vector. This comparative Southern blot analysis will provide a way to visualize the number of independent insertions of plasmid/*ARG7* genes in the *C. reinhardtii* genome and it will complement the genetic analysis outlined in (d) above.

Task 2: Single-Organism, Two-Stage Biophotolysis and Hydrogen Production

Subtask 2.1: Physiological Approaches to Improve the Yield of H_2-production
To increase the yield of the successful *single-organism, two-stage hydrogen production process* in the green alga *Chlamydomonas reinhardtii,* a number of physiological/practical treatments will be applied. (i) Test whether the forward reaction of the *reversible hydrogenase* can be accelerated by purging H_2 dissolved in the growth medium upon periodic bubbling with inert gas. (ii) Design and test cell growth media that accentuate the metabolism of H_2 production. (iii) Identify the rate-limiting step in the H_2-production process.

Subtask 2.3: Investigation of the Halotolerant Green Alga *Dunaliella salina* in H_2-production
The green alga *Dunaliella salina* is suitable for scaleup of H_2-production in mass culture since it thrives under high salinity, a condition that prevents contamination by other microorganisms. The research will apply the recently developed H_2-production protocol in *Dunaliella salina.* The work will rigorously investigate the premise of the halotolerant *Dunaliella salina* in the process of photobiological H_2-production.

Subtask 2.3: BioHydrogen Genomics/Informatics

If funding permits, in the model green alga *Chlamydomonas reinhardtii* and *Dunaliella salina,* UC Berkeley will investigate the presence of homologous reversible hydrogenase genes, such as *CpI* (identified as the Fe-only hydrogenase in *Clostridium pasteurianum*) and the *hox* family of genes, and identified as the reversible hydrogenase genes in the cyanobacterium *Synechocystis* PCC 6803. There will be collaboration with Dr. Peter Lindblad of Sweden on the *hox* genes. This subtask is critical for its understanding of the mechanism of the above-mentioned H_2-production process.

A Two-Phase Photobiological Algal Hydrogen Production System – National Renewable Energy Laboratory

The objective of this project is to fully develop and optimize an innovative photobiological H_2 production system discovered in FY99. The system is based on the temporal separation of H_2 and O_2 production by the green alga *Chlamydomonas reinhardtii* in a new and independent effort to demonstrate a viable commercial H_2-production process in the mid-term time frame.

Initial research efforts under NREL lead will focus on the investigation of other conditions that may result in even faster, specific, and reversible inactivation of photosystem II O_2 evolution, and on improvements in the yield of H_2 production exhibited by the current system. More specifically, NREL will investigate whether additional physiological manipulations by themselves or in combination with its current procedures will accelerate the process of photosystem II inactivation, and whether exposure to high light, high levels of O_2, or high temperature may similarly affect this process. In order to improve the yields of the current system, experiments will be designed, initially, to determine the rate-limiting step of the process. Once the rate-limiting step in H_2 production by the two-phase system is determined, appropriate measures will be taken to alleviate it. For example, if it is found that the rates of H_2 evolution are inhibited by build-up of product (i.e., H_2 accumulation), NREL will investigate whether different green algal species perform better under the same conditions. Preliminary results indicate that the *Scenedesmus* D3 strain, in contrast to *C. reinhardtii*, will produce H_2 against one-atmosphere of pure H_2. This strain will be examined in detail.

The ultimate goal of this work is to develop a mid-term hydrogenase-based, H_2-production system that can lead to a viable commercial process before a single-organism, water-splitting system can be developed.

Task 1: Determine The Rate-Limiting Step Controlling Current H_2-Production Activity

Task 1 will address the following possibilities in detail: build-up of H_2 during the H_2-production phase, which, due to the reversible nature of the enzyme, limits the rate of the forward H_2-releasing reaction; competition for reductant between the normal photosynthetic CO_2-fixing system and the hydrogenase pathway, leading to lower rates of H_2 evolution; and limitations in the rate of mobilization of stored metabolites or transport of reductant to the photosynthetic apparatus (photosystem I).

Task 2: Optimize Process

Task 2 will examine such parameters as: using other physiological manipulations to speed up the switchover to anaerobic conditions; treating the cultures with high light intensity to more rapidly inactivate photosystem II activity; finding ways to eliminate the requirement of acetate of O_2 evolution; and examining the loss of collected H_2 gas due to a less than optimal gas collection design.

A Two-Phase Photobiological Algal Hydrogen Production System –
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Improve switching time by 20%				◆		

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3.1.2 Hydrogen Storage Research Projects

A key component of hydrogen R&D is the development of storage systems for hydrogen. Stationary storage systems are needed to provide hydrogen for electricity generation to complement intermittent renewable resources and to store off-peak energy for use during peak energy periods. Stationary storage systems will also needed at vehicle refueling stations. Safe, lightweight hydrogen storage systems are needed for storing hydrogen on-board vehicles. Program hydrogen storage R&D is being conducted using carbon structures as well as metal hydride systems. Storage tasks are summarized in Table 3.3.

Table 3.3
Hydrogen Storage Research

Goal: Demonstrate safe and cost-effective storage systems for use in stationary distributed electricity generation applications, and for on-board and stationary applications in non-attainment areas.

Category	Project	Researcher
Carbon Structures	Carbon Nanotube Materials for Hydrogen Storage	National Renewable Energy Laboratory
Metal Hydrides	Hydrogen Transmission/Storage with Metal Hydride Organic Slurry	Thermo Power Corporation
	Hydrogen Storage	University of Hawaii
	Hydride Development	Sandia National Laboratories
	Hydride Beds	Sandia National Laboratories
Physical Storage	High Pressure Conformable Hydrogen Storage for Fuel Cell Vehicles	Thiokol Propulsion
	Vehicular Hydrogen Storage Using Lightweight Tanks	Lawrence Livermore National Laboratory
	Advanced Thermal Hydrogen Compression	Ergenics, Inc.
	Insulated Pressure Vessels for Vehicular Hydrogen Storage	Lawrence Livermore National Laboratory

CARBON STRUCTURES

Carbon Nanotube Materials for Hydrogen Storage - National Renewable Energy Laboratory

Carbon single-wall nanotubes (SWNTs) consist of one cylindrical and closed graphite sheet without a seam and are therefore essentially elongated pores of nanometer dimensions. These carbon materials are unique in their ability to reversibly store and liberate hydrogen with small excursions in temperature and pressure about normal ambient values. This research program seeks to capitalize on the interaction between molecular hydrogen and these elongated pores to develop an adsorbent for hydrogen which will provide a safe, cost-effective, convenient, and energy efficient method for on-vehicle storage of hydrogen. Other non-SWNT carbon-based adsorption systems may also be investigated to evaluate their efficacy in comparison to the proposed SWNT system.

The goals of this project are to produce large quantities of nanotubes with selected diameters, lengths, chiralities, and orientations in a cost-effective manner; controllably access the sites which strongly and reversibly bind hydrogen so that the kinetics, thermodynamics, and capacity of hydrogen adsorption may be simultaneously optimized. The long term goal is to scale-up production of optimized materials to enable ambient temperature and pressure adsorption of hydrogen at energy densities specified by the Hydrogen Program Plan (6.5 wt % and 65 kg/m^3).

It is reasonable to consider the possibility of a room-temperature, atmospheric-pressure hydrogen storage system based on SWNTs. The next phases of this work are focused on deepening the understanding of how these materials work, and developing their hydrogen storage capabilities at larger scales.

Task 1: Optimizing and Characterizing H_2 Uptake and Discharge

NREL has developed new methods for cutting and opening SWNTs during the past year that are the subject of a recently filed record of invention (NREL ROI 99-44). NREL will continue to develop these and other methods to cut and activate SWNT materials for hydrogen adsorption and desorption. Although gram quantities of highly pure materials are now available, its cutting procedure is currently applied to small samples weighing a few milligrams. With these materials, however, NREL has demonstrated an uptake of 4 wt% on a total sample weight basis. During this fiscal year, NREL will scale-up its cutting procedure to match the bulk amount NREL can synthesize and purify. The effectiveness of the scale-up will be revealed in the gravimetric H_2

Carbon Nanotube Materials for Hydrogen Storage
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Optimizing & Characterizing H2 Uptake and Discharge						
Store 0.01 gm of H2 at 4 wt% and room temperature			◆			
Nanotube Production, Purification, & Characterization						
Achieve continuous production of nanotubes at 50% yield				◆		

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storage densities which will be measured by temperature programmed desorption (TPD) and thermogravimetric methods. The temperature dependence of H_2 uptake will continue to be explored by TPD. The overall goal is to concurrently maximize the gravimetric and volumetric energy densities in samples having a high SWNT content.

In order to optimize the performance of the adsorbent it is important to identify the location of the bound hydrogen, and the mechanism by which it is bound. Data derived from this work will aid theoreticians in their efforts to model its results and predict optimal material configurations. Early work from NREL demonstrated that hydrogen was physisorbed on the SWNT material and suggested that tubes had to be opened in order to gain access to the SWNT interiors. This conclusion was based on a detailed analysis of TPD data. NREL began to work on determining the nature and location of the bound hydrogen using techniques such as nuclear magnetic resonance, neutron scattering (in conjunction with Prof. Jack Fisher at University of Pennsylvania), isotopic exchange reactions, and infrared absorption spectroscopy. These investigations will specify the locations of the bound hydrogen within the SWNT assemblies and help NREL understand the operative binding mechanisms so that theoretical upper limits may be determined, and optimal configurations may be targeted.

Since gram quantities of SWNTs are now available due to dramatic advances in both the arc- and laser-based synthetic processes, it will be possible to obtain pressure-volume-temperature data from these materials this year. These measurements will enable the equilibrium hydrogen pressures to be measured as function of temperature for nanotube samples synthesized and treated under different conditions. This information will define the pressure and temperature parameters for the container which will be required to hold SWNT materials, and allow the effect of H_2 over-pressures on adsorption to be ascertained.

Several new type of carbon materials have been reported to adsorb large (and in some cases unbelievable) amounts of hydrogen. This year NREL will apply its expertise and perform a few key experiments to evaluate the accuracy of some recent claims.

Task 2: Nanotube Production, Purification, and Characterization

NREL has recently developed laser-vaporization methods that are capable of producing SWNTs at yields in excess of 50-70 vol %, and can now produce gram quantities. NREL will continue to work to understand the details of the synthesis mechanism so that the process may be scaled up. NREL has learned that variation in the conditions of the laser pulse, the target structure, and the temperature can alter the diameters of the produced tubes. These different diameter tubes give rise to different hydrogen adsorption characteristics, and an understanding of this relationship will lead to higher hydrogen storage capacities.

The synthesis work will require substantial characterization to assess the dimensions and quality of the SWNTs that will be produced. Raman spectroscopy, thermal gravimetric analysis, and transmission and atomic force microscopies will be used extensively. NREL’s work in production will be focused on two distinctly different approaches, both of which are focussed at understanding the production mechanism while also reducing the cost of producing the material. The eventual goal is the same as NASA’s for these materials: \$10/kg. In the first approach, NREL will continue to maximize production yield and rate with the laser-vaporization approach and compare pulsed to continuous-wave operation in order to develop control over the purity and diameters of the produced nanotubes. This work will also involve moving to higher synthesis temperatures. This process can be made to be continuous by introducing target material continuously. In a second approach, NREL will begin working on template-based chemical vapor deposition methods for continuous production of SWNTs. The work will synergistically interact with the Office of Science research project that was recently funded.

METAL HYDRIDES

Hydrogen (H_2) Transmission/Storage with Metal Hydride Organic Slurry – Thermo Power Corporation

Thermo Power Corporation, Advanced Technologies Group, is developing a new approach for the production, transmission, and storage of hydrogen. In this approach, a metal hydride/organic slurry is used as the hydrogen carrier and storage media. At the point of storage and use, a metal hydride/water reaction is used to produce high-purity hydrogen. An essential feature of the approach is the recovery and recycle of the spent hydride at centralized processing plants, resulting in low cost and, if the primary energy source is a hydrocarbon, the potential sequestration of the CO_2 produced. The approach has two clear benefits: it greatly improves energy transmission and storage characteristics of hydrogen as a fuel, and it produces the hydrogen carrier efficiently and economically from a low cost carbon source.

Task 1: Investigate Metal Hydroxide to Metal Hydride Conversion Process in Laboratory-Scale Experiments

The objective of this task is to investigate the metal hydroxide to metal hydride conversion process with laboratory-scale experiments. These experiments will be performed to confirm the feasibility of the key steps in the processes under consideration.

Task 2: Detailed Process Analysis and Metal Hydride/Organic Slurry Materials Evaluation

The objective of this task is to perform detailed analyses of the proposed Metal Hydride Organic Slurry Approach for transmission and storage of hydrogen. Detailed thermochemical analyses will be made of the processes under consideration.

Hydrogen (H_2) Transmission/Storage with Metal Hydride Organic Slurry
Thermo Power Corporation

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Investigate Metal Hydroxied Conversion Process						
Complete process analysis			◆			
Process Analysis and Materials Evaluation						
Complete laboratory tests			◆			
Bench-Scale Recycle Process Experiments						
Complete bench scale recycle experiments					◆	
Bench-Scale Slurry Pumping Experiments						
Demonstrate pumping capability				◆		
Hydroxide/Organic Slurry Separation Experiments						
Demonstrate separation and drying in laboratory				◆		
Engineering Design and Economic Evaluation						
Complete detailed process and economic analysis					◆	
Infrastructure Evaluation						
Complete infrastructure analysis					◆	

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Task 3: Bench-Scale Recycle Process Experiments

The objective of this task is to develop a bench-scale metal hydride recycle furnace and to conduct a series of experiments to gather data on the process and demonstrate its feasibility. This task is aimed at exploring in greater detail the process steps defined by tasks 6 and 7.

Task 4: Bench-Scale Slurry Production and Pumping Experiments

The objective of this task is to further develop and demonstrate slurry production and to pump the resultant slurry over a bench-scale test pipeline.

Task 5: Bench-Scale Metal Hydroxide/Organic Slurry Separation and Drying Experiments

The objective of this task is to develop a bench-scale metal hydroxide/organic separation and drying system.

Task 6: Detailed Engineering Design and Economic Evaluation

The objective of this task is to update the preliminary engineering design and economic evaluation of the process performed in Task 5 using the process evaluated in Tasks 7 and 9.

Task 7: Infrastructure Evaluation

The objective of this task is to analyze the complete infrastructure required for transmission and storage of hydrogen with the metal hydride/organic slurry approach and to develop a scenario for how this infrastructure could be implemented, based on the existing infrastructure in the U.S.

Hydrogen Storage – University of Hawaii

University of Hawaii plans to continue development of sodium aluminum hydride based hydrogen storage materials that contain catalytic additives. UH has found that $NaAlH_4$ undergoes rapid dehydriding at temperatures as low as 100 C upon homogenization with selected transition metal complexes. After an initial dehydriding/rehydriding cycle, the catalytically enhanced hydrides have been found to have stable, cyclable hydrogen capacities that are greater than 4.5 weight percent. These findings suggest the application of these materials as hydrogen carriers for onboard fuel cells. Recent studies of catalytically enhanced $NaAlH_4$ by Bogdanovic have shown that the plateau hydrogen pressures that occur during dehydriding at 80-150 C in the solid state are also compatible with a practical hydrogen storage system. The next step in the development of these materials as practical onboard hydrogen carriers is to produce a second generation of improved dehydriding/rehydriding catalysts.

Task 1: Aluminum-Transition Metal Catalysts

The dehydrogenation of $NaAlH_4$ is known to occur by a multi-step process involving the reactions seen in equations 1 and 2. During the past year, catalysts have been found for

$$3\ NaAlH_4 \ \text{---------->}\ Na_3AlH_6 + 2\ Al + 3\ H_2 \qquad (1)$$

$$Na_3AlH_6 \ \text{---------->}\ 3\ NaH + Al + 3/2\ H_2 \qquad (2)$$

both of the dehydriding reactions as well as their reverse. An improved catalyst for the first dehydriding reaction is required for a practical hydrogen storage material that delivers 3.8 wt % hydrogen at 80 ˚C, while an improved catalyst for the second dehydriding reaction is required for a practical hydrogen storage material which delivers 4.8 wt % hydrogen at 140 ˚C. The doping of $NaAlH_4$ with transition metal alkoxides and chlorides has now been explored extensively. Although these studies have yielded the array of catalysts discussed above, this approach is nearly exhausted and new sources of catalysts must be considered.

Mixed aluminum-transition metal alloys and hydride complexes are especially promising candidates for improved catalysts. In order to explore this possibility, the Institute for Energy Technology (Norway) has supplied UH with samples of TiAl alloys for testing. Also if funding permits, UH plans to prepare and evaluate transition metal-aluminum hydrido complexes such as $\{(C_5H_5)_2ZrH(\mu\text{-}H)_2AlH_2(NMe_3)\}$ and

Hydrogen Storage
University of Hawaii (UH)

Task Designation/ Milestone		2000				2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Aluminum Transition Metal Catalysts						
Determine dehydriding kinetics of AlTi alloy	◆					
Synthesize transition metal-aluminum hydride complexes	◆					
Determine dehydriding kinetics			◆			
Solid State NMR Spectroscopic Studies						
Determine dehydriding activation parameters		◆				
Identify active catalysts in doped NaAlH4				◆		
Determine dehydriding activation parameters				◆		

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$\{(C_5H_5)_2Ti(\mu\text{-}H)_2AlH_2(THF)\}$ as catalyst precursors. Small amounts (~2 mole %) of the alloys and complexes will be introduced into bulk $NaAlH_4$ through ball milling techniques under an inert atmosphere. If funding permits, the dehydriding kinetics of the resulting materials will be determined by monitoring the evolution of hydrogen gas by volumetric methods. Materials which undergo faster dehydriding than Ti and/or Zr doped $NaAlH_4$ will be further studied by thermal gravimetric analysis (in collaboration with Prof. D.K. Ross, University of Salford) and solid state NMR spectroscopy (see below) in order to accurately determine the activation parameters of the dehydriding reactions.

Task 2: Solid State Nuclear Magnetic Resonance Spectroscopic Studies

Little is known about the catalytically active species in the doped hydrides. Clearly, UH's efforts to develop advanced catalysts would be greatly aided if the active catalysts in the doped hydrides were definitively characterized. If funding permits, UH hopes to accomplish this through solid state nuclear magnetic resonance (NMR) studies of the doped hydrides. This investigation will be conducted in collaboration with Prof. M. Conradi of Washington University and Prof. K. Kumashiro of the UH Department of Chemistry who are experts in solid state NMR spectroscopy. Prof. Conradi has developed methods whereby small (1-2%) amounts of hydrogen in defect sites can be observed from the bulk hydrogen in hydrides. Therefore, it should be possible to detect any transition metal complex hydrides present in doped $NaAlH_4$. The initial method development will be carried out at Washington University on samples of $NaAlH_4$ that are loaded with complex hydrides. Once methods have been developed, investigations on the doped hydrides will be carried out at UH utilizing the solid state NMR spectrometer that was provided to UH by the DOE several years ago through the University Research Instrumentation Program.

If funding permits, UH also plans to supplement its studies of the dynamics of the dehydriding of doped $NaAlH_4$ through solid state NMR spectroscopy. While the kinetics of the dehydriding process can be determined through quantification of the eliminated hydrogen gas or through thermal gravimetric analysis, these methods do not give direct information about the rates of the individual reactions seen in equations 1 and 2. UH plans to monitor the dehydriding and rehydriding processes by ^{27}Al, ^{23}Na and ^{1}H NMR spectroscopy at temperatures ranging form 100-150 ˚C. Since each of the hydride species will be directly observed and quantified over the course of the dehydriding and rehydriding processes, UH can determine the activation parameters for the both of the dehydriding reactions and the reverse rehydriding reactions. This information will provide better understanding of the catalytic effects resulting from Ti, Zr, and/or Fe doping and allow UH to better evaluate the relative effectiveness of the new catalysts that will be studied this year.

Hydrides Development - Sandia National Laboratories (SNL)

NO INPUT RECEIVED

Hydride Beds - Sandia National Laboratories

NO INPUT RECEIVED

PHYSICAL STORAGE

High-pressure Conformable Hydrogen Storage for Fuel Cell Vehicles - Thiokol Propulsion

On-board high-pressure storage of hydrogen for fuel cell powered vehicles presents a number of technical and economic challenges. Because the energy density of hydrogen is significantly less than that of conventional fuels, larger tanks are required for equivalent range. Furthermore, the geometry of traditional high-pressure cylinders generally does not conform to the available space on the vehicle, resulting in tank packaging issues. Tank cost and weight also have significant influences on the amount of fuel that can be carried.

Thiokol is addressing these issues through the development of high-pressure conformable tanks for on-board hydrogen storage. The lightest-weight approach uses high-strength filament-wound carbon fiber composite for structural efficiency, with plastic liners to act as permeation barriers. Thiokol’s conformable storage concept uses multiple cells, with the number and shape of the cells tailored to maximize internal volume within a rectangular envelope while maintaining membrane loading for structural efficiency. Each cell is filament wound with a combination of hoop and helical layers, followed by a hoop overwrap over the assemblage of cells. Depending on the shape of the envelope, up to 50% more storage is possible with a conformable tank than with cylinders.

The full-scale tank under development is a two-cell configuration fitting in an envelope 12.8 in. x 21.2 in. x 27.9 in., with a capacity of 3.4 lb. of hydrogen. The conformable tank provides 23% more capacity than two cylinders in the same volume envelope. An optional third cell would increase the tank width to 29.6 in., and the capacity to 4.8 lb. of hydrogen. Tank envelopes are consistent with space constraints on Ford’s P2000 fuel cell vehicle.

The tank is designed to a service pressure of 5,000 psi, with a burst safety factor of 2.25 consistent with existing standards for high-pressure vehicle fuel tanks.

High-pressure Conformable Hydrogen Storage for Fuel Cell Vehicles
Thiokol Propulsion

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Lot 1 Fabrication and Testing						
Evaluate & select liner materials	◆					
Fabricate 6 lot 1 Tanks		◆				
Complete qualification testing		◆				
Complete evaluation, design & process modifications		◆				
Lot 2 Fabrication and Testing						
Fabricate 6 lot 2 tanks			◆			
Complete qualification testing			◆			
Review final data				◆		

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Task 1: Phase II - Qualification Safety Testing

Successful completion of Phase I demonstrated the primary functional requirement for a full-scale high-pressure conformable hydrogen tank: the capability for safely withstanding the service pressure of 5,000 psi. However, additional requirements must be satisfied in order to demonstrate safe and reliable operation of the tank within the motor vehicle environment. Over a lifetime of service, the tank will experience cyclic loading due to repeated fills, extremes of temperature, exposure to corrosive fluids, potential damage both during handling and vehicle operation, and possible creep and stress rupture due to sustained high pressure loading.

The ANSI/AGA NGV2 standard provides a comprehensive set of design and qualification test requirements for compressed natural gas (CNG) vehicle fuel tanks to ensure safe operation over their lifetime. In the absence of a comprehensive standard for hydrogen vehicle fuel tanks, and because of their similarity with CNG tanks, Thiokol will use NGV2 qualification requirements as the basis for safety and durability testing and evaluation under the present program.

The primary objective of the Phase II effort is to subject tanks produced using the technology developed in Phase I to qualification testing based on NGV2 in order to identify and address critical safety and durability issues.

Subtask 1.1: Lot 1 Fabrication and Testing
One primary liner material and one alternate will be selected, based on the ongoing liner material evaluation testing, for the tanks fabricated for qualification testing. Currently, cross-linked polyethylene and polyvinylidene fluoride are the leading candidates, with Nylon-12 still being evaluated. Six full-scale tanks will be fabricated using the final design, materials, and processes developed under Phase I.

These tanks will be subjected to critical qualification safety and durability tests based on NGV2 qualification requirements for CNG tanks. These tests will include: pressure cycling at ambient temperature; drop testing; flaw tolerance testing; bullet penetration; accelerated stress rupture; and environmental testing, including gravel and pendulum impact, exposure to corrosive fluids, and high and low temperature exposure. While these tests do not represent the complete set of qualification tests under NGV2, they are regarded as the most critical in the present application.

The performance of the six tanks in the above tests will be carefully evaluated. Problem areas will be addressed through further testing, potentially leading to modifications to the materials, design, or processes to improve performance.

Subtask 1.2: Lot 2 Fabrication and Testing
A second lot of six tanks will be fabricated, incorporating the modifications resulting from the Lot 1 test and evaluation. Critical qualification tests will be repeated to assess effects of the modifications on tank performance. Tests that are determined not to be critical may be eliminated, with alternate tests substituted. These may include permeation, bonfire, or pressure cycling with hydrogen or natural gas.

Vehicular Hydrogen Storage Using Lightweight Tanks – Lawrence Livermore National Laboratory

Regenerative Fuel Cell (RFC) systems have been proposed and investigated sufficiently to gage their advantages for a variety of applications (portable, vehicular, utility, aerospace, etc.). Delivering predicted performance levels from RFC systems is much more arduous. Two key advanced component technologies that enable advanced RFC systems are undergoing rapid evolution: PEM cell stacks and lightweight composite hydrogen tanks. This proposal advances hydrogen tankage beyond the current state-of-the-art in the specific energy performance targeted by the DOE2000 goals and will provide tankage for demonstration vehicles.

Tanks with sufficient performance to meet the DOE 2000 goals for vehicle tankage have recently been prototyped by the LLNL team under DOE FY99 funding. The tooling and subcontractor preparedness already put in place by this effort provides a significant opportunity for DOE to obtain adequate hydrogen storage to demonstrate a variety of alternative vehicles. That opportunity will be pursued on the fast track required to integrate with DOE demonstration vehicles by advancing from two tank size directions: 18" (46 cm) O.D. x 48" (122 cm) length tankage already prototyped and a new diameter in multiple lengths (to be determined, although at present proposed to be12" (30 cm) O.D. with variable lengths, up to ~108"

Vehicular Hydrogen Storage Using Lightweight Tanks
Lawrence Livermore National Laboratory

		2000				**2001**
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Continued Prototyping and Burst Testing						
Complete 18" prototyping run		◆				
Burst test first 18" tank		◆				
Perform integrated leak test				◆		
Tooling and Prototyping of Multiple Length 12" Tanks						
Design and specify tooling			◆			
Prototype first generation of 12" tanks					◆	
Test burst pressure and pre-test for NGV-2						◆
Development & NGV-2 Certfication - 18" tanks						
Prototype second generation tank				◆		
Pre-NGV/2 test second generation					◆	
Replicate and NGV/w certify						◆
Permeation Inhibing Coating						
Specify test ariticles & processes		◆				
Deliver test articles by contractor				◆		
Collect permeation data				◆		
Development and NGV-2 Certification - 12" Tanks						
Build 2nd generation						
Perform NGV-2 risk reduction tests						
Replicate and NGV-2 certify 2n generation articles						
Design of FutureTruck						
Design FutureTruck tank				◆		

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(274 cm). The new tank size will be determined in collaboration with the Nevada Fuel Cell Bus Program, the FutureTruck Program, and Directed Technologies, Inc.

LLNL staff will work with external contractors who can provide experimental and prototyping capabilities. Indeed, it is necessary to work with tankage development contractors because of the intricacies of NGV-2 certification and the rigors of safely containing kilograms of hydrogen in experimental composite pressure vessels. Southern Research Institute (SRI) has a facility that was upgraded to deliver the unique capability to investigate hydrogen permeation through candidate liners at differential pressure up to 5000 psi (34.5 MPa). A continuation of materials testing at SRI is anticipated and would provide the opportunity to complete a preliminary survey of plastics (possibly coated) that might make sense for hydrogen tank liners.

Prototyping, testing, and certification of the two tanks sizes will be done. The certification process requires fourteen copies of a frozen design, which must be sent through a battery of tests at an experienced subcontractor (likely to be PowerTech). It does not make sense to replicate such a large quantity of tanks until a design with high likelihood of passing all NGV-2 tests has been frozen. Roughly double the production quantity (14) of tanks are anticipated to be necessary through two generations of risk reduction in order to make best use of the costly NGV-2 certification process.

As part of the solicitation, the LLNL team will attempt to provide the flexibility in specifications required for multiple tankage fabrication contractors to bid on the anticipated DOE solicitation. If several commercial organizations respond adequately to the anticipated solicitation, the two sizes being developed could provide the basis for issuing two contracts, each for more than half of a single contractor effort.

Only slight savings would be realized (~20%) by trimming this proposal to develop a single tank size. Three generations of risk reduction are planned, with only the second and third being replicated fourteenfold to commence NGV-2 certification. By using existing molds, the tooling for the new (~12" [30 cm] O.D. x up to ~108" [274 cm] long) size can proceed in parallel with the first generation of risk reduction. This first generation is likely to wrap up with roughly six fabricated tanks, and will occur in parallel with the deferred burst testing of the 18" prototypes that were deobligated in FY99. The second and third generations can also occur in parallel, at two different contractors each working on a different size, without significant additional cost. The likelihood of passing NGV-2 certification would decrease in this two-contractor scenario, since the knowledge obtained on risk reduction at one fabrication house may only be partially applicable to the other.

Task 1: Continued Prototyping and Burst Testing of 18" Diameter Tanks

LLNL will complete the prototyping run and burst testing for the 18" lot. The lab will also perform a integrated leak test.

Task 2: Tooling and Prototyping of Multiple Length 12" Tanks

LLNL will design and specify tooling. If funding permits, prototyping of the first generation of the (shortest and longest) 12" tanks will be completed. A test burst pressure and pre-test for NGV-2 will be conducted.

Task 3: Continued Development and NGV-2 Certification of (2nd generation) 18" Diameter Tanks

LLNL will build 2nd generation 18" diameter tanks. Pre-NGV-2 testing will be performed. LLNL will replicate and NGV-2 certify 2nd generation articles.

Task 4: Permeation inhibiting coatings - process development and testing

LLNL will specify test articles and processes. The lab will deliver test articles and add coated test articles to SRI permeation data collection. LLNL will also coat and improve full-scale liners.

Task 5: Continued Development and NGV-2 Certification of (2nd generation) 12" Diameter Tanks

If funding permits, LLNL will build 2nd generation 12" diameter tanks and perform NGV-2 risk reduction tests. The lab will also replicate and NGV-2 certify 2nd generation articles.

Task 6: Design for FutureTruck - Information Capture, Sizing Tradeoffs, Team Interfacing

If funding permits, LLNL will interface with FutureTruck team members.

Advanced Thermal Hydrogen Compression – Ergenics, Inc.

One obstacle impeding the development of economical hydrogen production, storage and utilization is hydrogen compression. Large mechanical hydrogen compressors have a high capital cost, consumer substantial amounts of energy and require frequent maintenance. Ergenics intends to develop an advanced thermal hydrogen compressor that can be powered by either waste heat from a hydrogen production process or solar hot water. The compressor would be used in conjunction with physical storage or other advanced storage system that requires hydrogen to be supplied at elevated pressure. The advanced thermal compressor has overwhelming advantages compared to mechanical hydrogen compressors, including smaller size, no moving hydrogen seals, nearly silent operation, and lower capital, operating and maintenance costs.

Ergenics has been producing hydrogen compressors for more than 15 years. Hydrogen is compressed using thermal energy in a metal hydride absorption system. In the thermal compressor, hydrogen is absorbed in a reversible metal hydride alloy at low pressure in a water-cooled container. The hydride alloys are active metal powders that are affected by gaseous impurities. Certain active gas species, such as water vapor, oxygen and carbon monoxide can gradually poison the alloy, reducing its hydrogen absorption capabilities. In the early 1990s, corrosion resistant alloys were developed for nickel-metal hydride batteries. Ergenics has invented and patented a process that enables hydride alloys to store hydrogen saturated with water vapor.

Ergenics will evaluate which impure gas species are likely to be present in hydrogen produced from advanced low cost production techniques and determine how to best mitigate their effect on thermal compression. Impurity effects on hydrides will be determined from Ergenics in-house database, published literature, and samples test in the laboratory. Availability of waste heat energy may be available from the various production processes will be assessed. A preliminary design and cost estimate for a service station sized thermal compressor of 2,000 scfh capacity will be performed. A life cycle analysis comparing capital, operating and maintenance costs with mechanical compression will be completed.

Task 1: Determination of Characteristics

Ergenics, Inc. will investigate the anticipated hydrogen characteristics expected from renewable energy production processes, including thermocatalytic, biomass, microorganisms and photolytic methods. Characteristics include gas composition, flow rates, pressure, and temperatures.

Advanced Thermal Hydrogen Compression
Ergenics, Inc.

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Task 3: Impurities Evaluation:

Ergenics, Inc. will analyze the effect of impurities on reversible metal hydride alloys. Predict alloy behavior absorbing different gas compositions. Resources used during this task will be Ergenics's internal database, published literature, and possibly, laboratory tests.

Task 4: Limiting Conditions of Operation:

Ergenics, Inc. will determine the limiting conditions of operation for the various gas streams based upon predicted alloy bed behavior.

Task 5: Application Selection

Ergenics, Inc. will select on application with the most promising combination of gas composition and heat availability.

Task 6: Process Flow Diagram

Ergenics, Inc. will produce process flow diagram, preliminary size calculations and cost estimate for a thermal compressor sized for service station duty that can be compared with compressors now used in conjunction with steam reforming of natural gas.

Task 7: Economic Analysis of Hydride Compressor

Ergenics, Inc. will perform an economic analysis of a hydride compressor compared to a mechanical compressor. Include capital cost, energy consumption, operating, and maintenance costs.

Task 8: Scope of Work for Phase II

Ergenics, Inc. will prepare the scope of work for Phase II activities necessary to lead the demonstration of advanced thermal compression.

Insulated Pressure Vessels for Vehicular Hydrogen Storage – Lawrence Livermore National Laboratory

The purpose of this project is to design, analyze, construct and test low temperature, high-pressure gaseous hydrogen storage vessels. These vessels should be capable of handling temperatures as low as 20 K and pressures as high as 34.4 MPa (5000 psi). These vessels have packaging characteristics similar to those of conventional low-pressure liquid hydrogen tanks, with much reduced venting losses. Compared with liquid hydrogen, cryogenic high-pressure hydrogen gas gives increased flexibility to the fueling infrastructure, since the vehicle can be fueled with liquid hydrogen, with high-pressure hydrogen cooled with liquid nitrogen, or with ambient-temperature hydrogen. Other forms of hydrogen storage exist, but they have limitations. Hydride storage is heavy, and compressed hydrogen requires a large volume.

This project aims to develop and demonstrate a near-term storage technology that can satisfy light duty vehicle storage needs in a cost effective way. This high pressure, low temperature vessel can be used in light duty vehicles, storage 5 kg of hydrogen and resulting gin a long range (640 km, 400 miles), low weight (30 kg, 66lb), and low external volume (140 liters, 37 gallons), and no hydrogen losses due to venting under all but the most extreme conditions. Other advantages of insulated pressure vessels include the following:

- Reduces the total requirement for liquid hydrogen because there is potential to use ambient-temperature, compressed hydrogen under most conditions. Liquid hydrogen may only be used when a long range is required.
- Decreases insulation requirements from those of a liquid hydrogen tank. This reduces the cost and thickness of the insulation. As a result, the external volume of a cryogenic pressure vessel is likely to be lower than the external volume of a conventional liquid hydrogen tank.

Insulated Pressure Vessels for Vehicular Hydrogen Storage
Lawrence Livermore National Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Construction of Insulation for Pressure Vessel						
Construct pressure vessel with insulation	◆					
Test insulated pressure vessel		◆				
Finite Element Analysis						
Conduct finite element analysis of pressure vessels				◆		
Full-Size Pressure Vessel Insulation						
Design insulation for full-size tank					◆	
Certification of Pressurized and Cryogenic Pressure Vessels						
Prepare test for vessel certification					◆	
Industrial Partners						
Partner with industry					◆	

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Task 1: Construction of Insulation for Pressure Vessel

Insulation for a pressure vessel will be constructed. The vessel will have MLVSI insulation and instrumentation to measure pressure, temperature and liquid level.

Task 2: Finite Element Analysis

A finite-element analysis of the pressure vessels will be performed to calculate the thermal stresses. The experimental information collected during this year will help in validating the model, evaluate alternative improved vessel designs, and determine possible failure modes.

Task 3: Insulation Performance

The insulated pressure vessel will be tested to determine insulation performance, and to calibrate the pressure, temperature and level instruments.

Task 4: Full-Size Pressure Vessel Insulation

Insulation for a full-size pressure vessel (90 liters internal volume) will be designed and built.

Task 5: Certification of Pressurized and Cryogenic Pressure Vessels

Tests listed in the DOT, SAE, and NFPA standards will be conducted for certification of pressurized and cryogenic pressure vessels.

Task 6: Industrial Partners

Industrial partnerships will be formed for developing a demonstration project that includes insulated pressure vessels.

3.1.3 Hydrogen Utilization Research Projects

Utilization of hydrogen as an energy source occurs typically either via an electrochemical process such as in a fuel cell or by a combustion process. In addition, the use of hydrogen necessitates the ability to detect its presence in the event of leaks. The Hydrogen Program effort also supports R&D in the area of hydrogen sensors. This section, summarized in Table 3.4, is categorized accordingly.

Table 3.4
Hydrogen Utilization Research

Goal: Develop fuel cell and reversible fuel cell technologies as an efficient low-cost means of converting hydrogen into electric power.

Category	Project	Researcher
Fuel Cells	The Corrosion of Metallic Components in Fuel Cells	National Renewable Energy Laboratory
	Small Battery/ Fuel Cell Alternative Technology Development	Los Alamos National Laboratory
	PEMFC Stacks for Power Generation	Los Alamos National Laboratory
	Low Cost Reversible Fuel Cell System	Technology Management, Inc.
	Hydrogen Delivery System to PEM Fuel Cell	New Jersey Department of Transportation
	Gallium Nitride Integrated Gas/Temperature Sensors for Fuel Cell System Monitoring for H_2 and CO	Peterson Ridge, LLC
Internal Combustion Engines	Internal Combustion Engines Research and Development	Sandia National Laboratories
Hydrogen Safety	Thick Film Hydrogen Sensor	Oak Ridge National Laboratory
	Interfacial Stability of Thin Film Hydrogen Sensors	National Renewable Energy Laboratory
	Dispersion of Hydrogen Clouds	University of Miami
	Development of Codes and Standards from the Safe Use of Hydrogen	National Hydrogen Association
	Integrated Micro-Machined Hydrogen Gas Sensors	Advanced Technology Materials, Inc.

FUEL CELLS

The Corrosion of Metallic Components in Fuel Cells - National Renewable Energy Laboratory

When one is considering the mass production of fuel cells, the manufacturability of each component is very important. To obtain the economy of mass production, approximately one million fuel cell systems need to be manufactured each year, that is almost 100,000 per month. Assuming 120 bipolar plates per stack, that is 12 million bipolar plates per month or 400,000 per day! That means these plates must be injection molded or stamped from metal stock. Because of the need for high conductivity, metal stock is a good possibility. However, when considering metal stock, a number of problems arise from the possibility of corrosion leading to failure of the stack. Because of the unique and complex environment in a fuel cell stack, the importance of corrosion testing cannot be understated. A fuel cell stack has a humid environment that includes both oxidizing and reducing atmospheres, small amounts of fluoride leach from the membrane, and other halides, as well as SOx, and NOx are available from the atmosphere. These conditions can interact in a complex way to attack the metal plates leading to corrosion. Additionally, if the metal plates contain iron, it can leach out into the membrane blocking the sulfonic acid sites, thereby reducing the conductivity of the membrane. Iron can also act as a catalytic poison to degrade the membrane.

The goal of this research is to determine corrosion mechanisms for various metal alloy compositions, and to develop techniques for long term corrosion protection for thin metal foils.

Task 1: Conducting Metal Oxides for Corrosion Protection of Metal Bipolar Plates

The usual way in which stainless steels and titanium are protected is use of an inert oxide coating that naturally forms on the surface. Unfortunately, these oxides are typically insulating, leading to ohmic losses within the cell. If these oxides could be made conducting, then perhaps they would not only protect the underlying metal plates from corrosion, but also provide a conducting pathway for the flow of current.

NREL is unique in having significant experience in conducting oxides based on their use in various types of solar cells. For example, conductive tin oxide, used as the current collector for solar cells, may offer the appropriate protection and give high conductivity. This includes SnO:F which would likely be stable in the presence of fluoride. Other coatings of interest are ITO (indium tin oxide), ZnO and SnO_2. Tungsten trioxide, used in electrochromic devices, becomes conducting in the presence of hydrogen and perhaps could be used as a protective coating for the hydrogen side of the plate. In solar cells, these

The Corrosion of Metallic Components in Fuel Cells
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Conducting Metal Oxides for Corrosion Protection						
Report on stability in the presence of F-, SOx, Cl-					◆	
Plasma Treatments for Passivation of Plates						
Report on stability of N plasma treatment for stainless steel				◆		

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coatings are deposited on glass and on stainless steel in large areas and at high volume. For this work, NREL would combine its expertise in corrosion testing with its unique capability in conducting oxides.

Task 2: Plasma Treatments for Passivation of Metal Bipolar Plates

It is known that exposing metals to various types of gas plasmas can greatly alter the chemical characteristics of the surface. Imbedded ions such as nitrogen and hydrogen can permanently alter the reactivity of the interface. It may be possible to provide corrosion protection by simply cleaning the metal components in a gas plasma. NREL has the facilities for treating metal components in various gas plasmas.

Small Battery/Fuel Cell Alternative Technology Development - Los Alamos National Laboratory (LANL)

The appearance this past year of several conferences emphasizing portable power applications for fuel cells reflects the burgeoning interest in this potentially enormous market niche. In this program, LANL is partnered with DCH, Inc., in a Cooperative Research and Development Agreement (CRADA) to develop a unique low-power portable fuel cell and system for applications that require a combination of reliability, simplicity and low-cost. The advantage of this fuel cell system over current competing designs is that it does not require the use of peripherals such as cooling or reactant flow fans and can operate effectively with no active humidification, no active cooling, and no pressurization or forced flow of the cathode air. The system is inherently stable and self-regulating. A passive scheme is used that relies on diffusion limited oxygen access to maintain a positive water balance. The oxygen in the air must diffuse into the stack from the periphery of the flow-field plates. For this reason the stack is often described as "air-breathing." Given that the oxygen must diffuse in, twice as much water (as there are two molecules formed per O_2 that reacts) must diffuse out to maintain an even balance. While it first appears that a surplus of water is obtained, the fuel cell stacks quickly heat up and the water removal is greatly facilitated. Overall, the balance remains fairly even such that the polymer electrolyte membranes do not dry out, even at relatively high continuous operation temperatures (+60 C). Thus, the diffusion supply scheme results in simple stacks with reliable and stable performance. Since the oxygen needs to diffuse in from the periphery of the cathode flow-field plate, the fuel cell assumes a cylindrical configuration that utilizes circular flow-field plates with an annular hydrogen feed manifold and a single tie-bolt extending up through the central axis of the stack. With this geometry, the hydrogen supply to the unit cells is radially outward, and the air supply is from the periphery inward. This configuration facilitates performance (e.g., maximizes cooling surface area, air access, etc.) and is very simple for cost considerations (low parts count, all parts are radially symmetrical, etc.) has several advantages. To operate this type of fuel cell stack only a low pressure hydrogen supply is required which can be provided from a pressurized source (such as metal hydride canisters) via a compact low-pressure regulator.

Small Battery/Fuel Cell Alternative Technology Development
Los Alamos National Laboratory

		2000				2001	
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2
300 W Module Development							
Electronics/ RHS sensor integration				◆			
Fabricate stacks					◆		
Demonstrate module					◆		
Alternative Materials Development							
Develop and procure materials						◆	
Test components						◆	
Compact 2 W Module Development							
Design and test single cell				◆			
Test stack						◆	
Demonstrate module					◆		

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Task 1: 300 W Module Development

An important technical objective for the second year of this CRADA project is to continue the effort to design, fabricate and test modular air-breather fuel cell stack systems incorporating RHS technology for hydrogen monitoring and feedback control. The milestone is an eventual 300 W module containing the necessary electronics and RHS technology. A number of potential applications require some level of remote status monitoring and operability assurance.

Over the past year, a fair amount of effort was dedicated to optimizing performance, as was reflected in last year's tasks. The operation and performance contributions of the various components are now better understood and nice performance improvements were attained.

Task 2: Alternative Materials Development

This year, LANL intends to continue evaluating alternative materials but with cost as the primary priority. Now that DCH is attempting to commercialize the system, many of the component costs are uncomfortably high for many potential markets. For example, the backing materials that provide the best performance are quite expensive. In such cases, a small sacrifice in performance could conceivably be tolerated if the costs can be substantially reduced. Task 2 is then the investigation of cost-effective alternate materials. Many of the components, i.e., flow-fields, backings, cooling fin separators, could conceivably provide significant cost reductions.

Task 3: Compact 2W Module Development

Thus far, most of the air-breather development effort has concentrated on roughly 5 cm (2") diameter circular cells. While originally envisioned as having much smaller diameters (say C-battery size), the larger diameter was originally chosen to facilitate prototype development and is naturally more useful when 10's of watts are required. Recently, enormous interest has been expressed in power supplies for personal electronics, such as cellular phones, which require approximately 2 watts. For such applications, much smaller diameters would be of interest in order to accommodate the fuel cell and hydrogen supply in an equivalent size battery replacement pack. Unfortunately, it is difficult to obtain a reasonable fraction of active area with such small diameters because so much of the plate area is lost to seals, the tie bolt and the hydrogen feed region. New schemes are necessary to more effectively capitalize on the available area and will be developed in Task 3. Other issues involve schemes to facilitate cooling with the higher current densities that will be obtained with the smaller diffusional pathway distances.

PEMFC Stacks for Power Generation – Los Alamos National Laboratories

Much of the interest in polymer electrolyte membrane (PEM) fuel cell development has been shifting from transportation to stationary power applications. In contrast to molten carbonate or solid oxide fuel cell technologies which are most appropriate for large-scale power applications, PEM fuel cells are envisioned for small, home-based power sources on the roughly 3 - 5 kW level. Plug Power, LLC, a fuel cell manufacturer, is primarily pursuing the development of such systems. Technological advances in PEM fuel cells at LANL are of potential utility for the development of readily manufacturable, low-cost and high performance fuel cell systems operating at near-ambient reactant pressures. As such, the two parties are entering into a CRADA to collaborate on addressing some of the more pressing issues. The primary tasks involve the investigation of both stainless steel and composite bipolar plates, CO tolerant anodes, and novel humidification and stack operation schemes.

One of the major limitations to commercialization is currently the bipolar plate technology. Historically, machined graphite plates have been the material of choice, but are clearly too expensive for mass production. The bipolar plates need to be highly electrically conductive, durable, impermeable and corrosion resistant, a surprisingly difficult combination to realize. Metal hardware is of interest because of its toughness and the versatile fabrication options, but corrosion is a significant difficulty. Previously in this program, LANL considered stainless steel (SS) alloys and have operated cells for as long as 2000 h using 316 SS with little evident effect, but the inclusion of metal ions into the membrane discourages operation on a much longer time frame.

Task 1: Metal Bipolar Plates

Since more like 40,000 h would be needed for stationary applications, continued work, in task "1", will concentrate on metal alloys that are more noble than 316SS yet are still relatively inexpensive. Also,

PEMFC Stacks for Power Generation
Los Alamos National Laboratories

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Metal Bipolar Plates						
Improve design of metal bipolar plates						
Composite Bipolar Plates						
Develop composites for bipolar plates			◆			
CO Tolerant Anodes						
Develop CO tolerant anodes				◆		
Novel Humidification and Ambient Pressure System						
Develop novel humidification			◆			
Develop ambient pressure system						
Stack Fabrication, Testing and Demonstration						
Fabricate and test stack					◆	
Demonstrate stack/fuel processor					◆	

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work will continue in collaboration with another company on a proprietary low-cost metal coating technology that is of a more speculative nature but has shown some promising preliminary results.

Task 2: Composite Bipolar Plates

As a whole, the metal-based based bipolar plate approach is more of a long-term solution because of the various corrosion difficulties and the need for extensive testing before implementation. For the shorter term, LANL has been working with Plug Power in the development of composites based on a LANL approach that have already shown substantial promise in single cell and short stack testing at Plug Power. Further development and testing of these materials will continue in task "2".

Task 3: CO Tolerant Anodes

Operating a home-based system on natural gas will require a fuel processor to provide hydrogen to the fuel cell. The reforming and/or partial oxidation fuel processor reactions produce byproducts such as CO and CO_2. If the CO is not removed from the fuel stream in some manner before it reaches the fuel cell it will severely affect performance, especially with standard anode designs. The typical strategy is to remove the CO through a series of additional steps, but removing the last tens of ppm's can not always be routinely assured with typical systems. Therefore, anodes that can tolerate higher levels of CO than conventional electrodes are of interest to withstand excursions that may occur with start-up of the fuel processor or during variations in load levels. A related issue is the supply pressure of the reformed fuel. Since domestic natural gas is typically delivered into the house at less than 1 psig, the preferable option to compression may be to operate a low-pressure fuel processor. In this case, the fuel cell anode will also then need to operate at near ambient pressures. Task "3" is to continue work on anodes that are designed and optimized for both low-pressure operation and CO tolerance.

Task 4: Ambient Pressure System Development

Near ambient pressure operation is of interest for the air or cathode side for much the same reason as the anode side, that is, to minimize parasitic power losses and lower the component costs. If pressures can be kept low, a blower can be used to provide the air flow through the fuel cell. While not particularly efficient, a blower is obviously much less expensive than a turbine or positive displacement compressor, and with very low pressures, the PV work required is minimal and the device efficiency is not much of a factor. Since the cathode kinetics are roughly first order with respect to oxygen partial pressure, the stack power densities are not as high as with the pressurized cells, however, it can be shown that once the parasitic losses are taken into account, the net power densities are not very different. A number of issues arise with very low-pressure operation. Low pressure operation often results in drier operating conditions due to both lower current densities (less water produced) and the higher water vapor volume fractions (more water removed with the air effluent compared to pressurized). As such, the effectiveness of the membrane hydration scheme becomes more significant at the lower pressures.

Task 5: Novel Humidification

Direct liquid water hydration of the membranes then appears to have advantages over the classical means of cell hydration, namely, reactant humidification. Avoiding reactant humidification also eliminates the pressure drop required to force the reactant air through the humidification module, which further decreases the parasitic power requirements. As such, major areas of emphasis are direct liquid membrane hydration and near-ambient system schemes which are addressed in tasks "4" and "5", respectively.

Task 6: Stack Fabrication and Testing

Finally, the ultimate objective represented by tasks 6 and 7 is the demonstration by industry of a 3 – 5 kW system integrated with a fuel processor that incorporates LANL technologies.

Task 7: Stack/ Fuel Processor Demonstration

Due to Plug Power's aggressive development and production timetables, it can be appreciated that not all of these tasks will be manifested in the demonstration. For example, the metal hardware is a more speculative and longer term technology and hence is not expected to make it into the demonstration system. However, because of its potential, LANL will continue to work on the issue with its industrial partners in anticipation of future products.

Low Cost Reversible Fuel Cell System – Technology Management, Inc. (TMI)

A solid oxide fuel cell (SOFC)-based system utilizes a solid electrolyte operating at high temperature to electrochemically convert gaseous fuels (hydrogen and mixed gases) and oxygen to electricity. Unlike polymer electrolyte membrane (PEM) fuel cells and alkaline fuel cells, SOFCs do not require electrolyte management, have very fast electrode kinetics, and can be configured into systems from under a kilowatt up to multi-megawatts. SOFCs are potentially very reliable, compact, and noiseless. They can produce a high-grade heat by-product and have high system efficiencies. The electrolytic counterpart is a solid oxide electrolyzer (SOE); a fuel cell which operates in reverse. A voltage is applied across the solid electrolyte at high temperature to electrolyzer steam into hydrogen and oxygen. Because market opportunities for SOE systems are relatively small compared to the SOFC, SOE development is neither as advanced nor as widely pursued as SOFCs.

The reversible fuel cell system proposed is based on the use of TMI SOFC technology developed for fuel cell and/or electrolyzer operation in conjunction with hydrogen storage technologies developed by Sandia National Laboratories. The use of the TMI sulfur-tolerant SOFC technology allows system designs with a broader range of applications to be considered; the systems to be examined will work not only hydrogen produced through electrolysis, but will have the capability to reform and operate directly on renewable energy sources, such as biogas, and conventional energy sources, such as diesel or propane, both of which may contain significant concentrations of sulfur contaminants.

Phase I study will determine the conceptual designs and operating conditions for the TMI reversible fuel cell system and hydrogen storage system that combine high net energy-storage efficiency with low capital costs. Two different approaches will be evaluated for the reversible fuel cell/electrolyzer system: a single, dual-purpose stack which operates in both electrolysis and fuel cell modes; and two single-purpose stacks, one operating as an electrolyzer and one as a fuel cell. The first approach may produce the simplest system, using fewer system components, but will require greater control complexity. The second approach will allow the use of components optimized in the respective operating regime and therefore may produce better overall performance, with better potential for lower life cycle costs. Because there are multiple interactions between the reversible fuel cell and the hydrogen storage systems, the integration and operation of these two systems will be examined in detail.

Low Cost Reversible Fuel Cell System
Technology Management, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Preliminary Design Studies						
Complete preliminary design studies		◆				
Cost Studies						
Complete cost studies			◆			
Phase II Plan Development						
Develop phase II plan				◆		

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Task 1: Select Boundary Conditions

In cooperation with Sandia National Laboratory, one or more sets of boundary conditions for reversible module and hydrogen storage operation will be selected, including temperatures, pressures, compositions, and flow rates. This will include details for using the fuel cell hot exhaust stream to liberate the hydrogen from storage. Also, one or more example values for the usable hydrogen storage capacity in standard cubic meters will be chosen.

Task 2: Preliminary Design Studies

Perform preliminary engineering design studies of the reversible modules for both modes of operation, including material and energy balances, chemistry and electrochemistry, heat transfer and fluid flow, high temperature gaseous diffusion, stress analysis, materials selection, and module auxiliaries. The studies will examine several alternative stack configurations and flow schemes, including both dual-purpose single stacks and individual electrolyzer and fuel cell stacks. Preliminary design schematics and flowsheets will be sketched. For each design, efficiency calculations will be performed versus percentage power for both modes of operation. Different types of supplemental fuels will be considered. Engineering studies for two different sizes of hydrogen storage systems will be performed.

Task 3: Cost Studies

Preliminary estimates will be made of installed capital costs and operating costs, with the target capital cost for the reversible fuel cell systems being under $1000/kW. Installed cost studies will be performed for the most attractive designs at two or more levels of annual production and at sizes from 500W to 3 kW. Preliminary installed capital and operating cost estimates will be made for entire energy systems. The cost studies will consider both installed capital cost and expected operating costs for selected example load profiles. All costs will be combined to produce average total costs per kWh of power delivered to the user for the various example cases.

Task 4: Prepare Phase II Development Plan

Phase II development work will lead to a complete prototype demonstration system, including a reversible fuel cell system, hydrogen storage system, water storage system, power conditioning system, load bank, and test instrumentation. The plans will include a detailed statement of work, timetable, cost breakdown, intermediate milestones, and final deliverables.

Hydrogen Delivery System to PEM Fuel Cells – New Jersey Department of Transportation

Hydrogen gas is currently the environmentally desirable fuel of choice for powering fuel cells. However, hydrogen gas that is stored in compressed gas cylinders that are heavy, bulky, and complicated with pressure regulators. The New Jersey Department of Transportation uses hydrogen gas stored in compressed gas cylinders to supply the needed hydrogen for hydrogen fuel cells. The main intent of this project is to evaluate water-based sodium borohydride as a replacement fuel. The proposed system will provide high purity hydrogen gas that can be safely generated on-site and stored in non-bulky containers, versus the current hydrogen gas system that uses heavy weight, highly pressurized steel cylinders.

The project will analyze the sodium borohydride alternative in the storage, transportation, use, and production of hydrogen gas; determine the necessary integration of the new fuel source with fuel cells; evaluate the cost benefit analysis of such alternative replacement; and produce a final specification for the new hydrogen fuel source if it is found acceptable.

Task 1: Rate and Yield Maximization

New Jersey Department of Transportation has identified several catalysts suitable for generation of hydrogen. These catalysts are robust and useful for a wide range of applications. The catalysts behave different under specific conditions and have different characteristics. These must be catalogued to determine the best catalyst, substrate and combination of fuel, and optimize reaction rates for a given application.

Task 2: Catalyst Production

New Jersey Department of Transportation will manufacture the current and new combinations of the catalyst. Millennium Cell will also optimize the production techniques in an economic manner to ease the transition to commercial scale-up.

Task 3: Construction of Hydrogen Generators

A series of hydrogen generators will be manufactured leading to the required size.

Hydrogen Delivery System to PEM Fuel Cells
New Jersey Department of Transportation

NO GANNT AVAILABLE

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Task 4: Technical Coordination and Planning

H Power will hold coordination and planning meetings with Millennium Cell to provide for exchange of ideas for hydrogen generator designs suitable for real-world fuel cell systems. Issues to be addressed include hydrogen generation rate, hydrogen capacity, system control, water and thermal management, and specific fuel cell integrated system configuration.

Task 5: Assessment of Hydrogen Generator Design and Performance Characteristics

H Power will observe hydrogen generator testing at Millennium Cell. Data will be analyzed and recommendations will be formulated for transmittal to Millennium Cell. These will relate to design characteristics and control strategies as these affect generator performance, in addition to prognosis for successful fuel cell integration.

Task 6: Integration and Testing of Small-Scale Hydrogen Generator in Fuel Cell System

H Power will work with Millennium Cell to select a suitable small-scale hydrogen generator concept for integration with a fuel cell system. The hydrogen generation rate and capacity will be determined and the commensurate H Power fuel cell system will be identified. H Power will integrate the generator performance and comparability will be monitored. After fine-tuning of the system is completed, H Power will acquire test data and evaluate generator characteristics. The results will be reviewed with Millennium Cell and recommendations will be made for follow work.

Gallium Nitride Integrated Gas/ Temperature Sensors for Fuel Cell System Monitoring for H_2 and CO – Peterson Ridge, LLC

The electrodes in a solid polymer electrolyte fuel cell systems demand hydrogen fuel free from carbon monoxide (CO), otherwise the platinum fuel cell electrodes are poisoned and fuel efficiency is degraded. Steam reforming of hydrocarbon fuels produces a mix of hydrogen, carbon dioxide, and enough by-produce CO to poison the electrodes. Preferential oxidation of CO to reduce this contaminant is accomplished over a noble metal catalyst typically platinum by adding oxygen to the hydrogen fuel upstream of the preferential oxidation catalyst. An inexpensive monitor to confirm the preferential oxidation system catalyst efficiency and control the system conditions is necessary to avoid the risk that preferential system catalyst degradation could lead to reduced fuel efficiency or failure of the fuel cell due to contaminated hydrogen. Since the environment for a preferential oxidation system monitor is rich in hydrogen, the problem is developing a sensor that can monitor carbon monoxide without the sensor output being dominated by hydrogen.

A successful Phase I program would yield a sensor that can monitor hydrogen and the primary catalyst poison, CO. The benefits of a successful sensor are fuel efficiency optimization and safe operation of polymer electrolyte fuel cell systems. Phase I tests the sensors in the laboratory. Phase II develops prototype monitors which can be field-tested.

Task 1: Fabricate Schottky Catalytic Metal Contacts in a MESFET Device

Schottky metals contacts to be used in this work ion gas microsensors include Pt, PdAg, and Rh. Fabricated Schottky contacts have been successfully fabricated that can withstand long term exposure to air ambient temperatures exceeding 500°C using Pt and Pd. Process technology has been used and developed that has resulted in highly adherent contacts that do not delaminate or peel off at high temperatures. In addition to the MESFET, single or multiple arrays of microfabricated Type K thermocouples will be incorporated onto individual GaN MESFET gas sensor circuit dies. Thermocouples will be protected by an inert dielectric. For reasons based on gas sensor performance, aluminum oxide will be the primary dielectric. The slotted electrode design is fabricated using a lift-off process. The lift-off process is a standard in many foundries and is more efficient with a high aspect ration of length to width as the metal thickness increases.

Gallium Nitride Integrated Gas/ Temperature Sensors for Fuel Cell System Monitoring for H_2 and CO
Peterson Ridge, LLC

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Fabricate Schottky Catalytic Metal Contacts						
Fabricate first catalytic gate MESFETs		◆				
Analysis for Mechanical and Electrical Integrity						
Analyze mechanical and electrical reliability			◆			
Surface and Interface Chemical Analysis						
Gas test in pure gas and simulated fuel			◆			

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Task 2: Analysis for Mechanical and Electrical Integrity

High temperature electronic characterization of contacts can be carried out in a dedicated ion- and cryp-pumped UHV chamber equipped with a residual gas analyzer and a 25 to 1000°C heater sample stage if needed. This system can be viewed as representing an ideal hermetically sealed package. Leak valves attached to the chamber will permit variable quantities of air, oxygen, nitrogen, etc. to be leaked into the chamber during the acquisition of in-situ electrical data such as resistivity and transmission line measurements. The chamber can be pressurized to greater than 1 atm using the leak valves for a complete and comprehensive set of electrical experiments on the temperature and pressure effe4cts of the Schottky and ohmic contacts to GaN that compromise the n-GaN MESFET under different ambient gases can be performed. High temperature I-V, C-V, and deep level transient spectroscopy can be performed on the GaN/Schottky barrier systems. A commercial Digital Instruments atomic force microscopy system is also available to characterize the GaN/contact systems. The temperature testing for mechanical stability will be carried out on a temperature-controlled chuck.

Task 3: Surface and Interface Chemical Analysis

Auger, XPS, and SIMS depth profiling will be routinely performed by the University of Utah in the ohmic and Schottky contacts which are exposed to automobile exhaust for prolonged periods of time at high temperatures. These contacts will also be analyzed using EDAX-equipped SEMs. Studies will be performed to understand possible degradation and failure mechanisms for these contacts to n-GaN due to high temperature, harsh environment exposure. Focused ion beam trenching and TEM and EDAX analysis scanning across freshly exposed interfaces will also be performed under a service contract to the Material Sciences Department of the Oregon Graduate Institute.

Task 4: Test Sensors for High Temperature Operation

Sensor test articles will be bonded to alumina supports with screen-printed contacts extending outside the furnace for electrical contact to power supply and signal processing electronics. Testing in simulated fuels will be done in a modified tube furnace at Fluence's facility. Four standard gas concentrations will be prepared in UHP nitrogen. These data will be collected with and without a background of MDL gas from all five cylinders. The temperature program will start at room temperatures an increase incrementally until the sensors lose sensitivity or fail mechanically. The sensors will be challenged with a stepwise addition of each gas separately, then challenge the sensors will all gases and simultaneously. Temperatures will be increased when the isotherms for each of the gases and mixtures have been determined. The gas exposure experiments will run continuously with increasing temperature until mechanical failure or loss of sensitivity occurs or the safety limit of the experiments is reached.

INTERNAL COMBUSTION ENGINES

Internal Combustion Engines Research and Development ─ Sandia National Laboratories

Internal combustion engine cycles are fundamentally capable of greater than 50% efficiency. In addition, the power output characteristics of an auxiliary power unit (APU) for a hybrid vehicle are different than for conventional cars. By rethinking the problem from a blank sheet a new approach has materialized.

The approach utilizes a free piston oscillating between two combustion chambers, and generating electricity directly from the oscillatory motion of the piston. Combustion occurs when a homogeneous fuel/air charge is compression heated to the point of reaction. In this way both rapid reaction rates, approaching constant volume combustion, and

Internal Combustion Engines Research and Development
Sandia National Laboratories

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Alternator Design						
Complete summary report of alternator design			◆			
Engineering Alternator Assembly and Fabrication						
Assemble prototype for testing			◆			
Test the Sandia Design Alternator						
Produce summary document of alternator performance				◆		
Test the Magnequench Alternator Design						
Produce summary document on alternator design				◆		
Model and Design Inlet and Exhaust Flow						
Model & design inlet and exhaust flow		◆				
Develop a Scavenging Model						
Develop port loop scavenged model			◆			
Measure Performance of the Scavenging System						
Design experiment to validate KIVA model			◆			
Demonstration of Performance of the Experiment						
Demonstrate performance of scavenging experiment				◆		
Performance of Key Scavenging Characteristics						
Measure key scavenging characteristics					◆	
Assess accuracy of the KIVA predictions					◆	
Sharing Alternator Development Data with CRADA						
Share alternator development with Caterpillar					◆	

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extremely lean mixture combustion, which essentially eliminates NOx formation, is realized. This appears to be the combustion approach that can achieve both high efficiency and low emissions, but still retain highly developed reciprocating engine technology and fuel flexibility required to transition to a hydrogen energy carrier society.

Since the fuel/air mixture, which is delivered premixed to the cylinder, is ignited by compression heating, the piston position at the time of combustion is determined by compression ratio and initial temperature. The free piston configuration provides a method for controlling the compression ratio electronically, thus allowing continuous optimization of performance and fuel flexibility.

The first goal of its research is to demonstrate the efficiency and emissions performance of a 30 kW generator in a research environment. Following this accomplishment will be refinement of the research unit into a fieldable unit for demonstration, coupled with a wind generator and used for generation when wind power is down.

To date the combustion characteristics of homogeneous charge compression ignition with a free piston have been demonstrated. Also, the design of the linear alternator which converts the piston oscillation to electrical energy is 70% finished. The tasks remaining are the fabrication and experimental characterization of the linear alternator, design and testing of the two-stroke cycle inlet/exhaust process, development of control system algorithms and hardware, diagnostics and startup processes.

Task 1: Alternator Design

Sandia will finish the alternator design, including the diagnostic capability. Sandia will complete the finite element model of the magnetic/ electrical aspects of the device, and produce a summary document of the optimization investigation.

Task 2: Alternator Assembly and Fabrication

Sandia will produce the engineering drawing of the alternator assembly and fabricte the parts. The prototype will be assembled for testing on the alternator tester previously developed.

Task 3: Test the Sandia Design Alternator

The alternator by itself will be driven through a 6-inch stroke at 40 Hz by a modified Caterpillar 3304 engine. Sandia will measure the electrical output of the alternator and the loads on the stator assembly to determine conversion efficiency. The lab will produce a summary document of the Sandia alternator performance.

Task 4: Test the Magnequench Alternator Design

Sandia will produce a summary document of the Magnequench alternator design.

Task 5: Model and Design the Inlet and Exhaust Flow

Sandia will model the inlet / exhaust flow of the combustion cylinder utilizing KIVA and will develop a design based on uniflow scavenging.

Task 6: Develop a Scavenging Model

Sandia will develop a scavenging model based on cylinder port (loop) scavenging.

Task 7: Measure Performance of the Scavenging System

Sandia will design an experiment to measure the performance of the scavenging system under specific conditions to validate KIVA predictions.

Task 8: Demonstration of Performance of the Experiment

Sandia will produce the engineering drawings of the scavenging system experiment and fabricate the parts. The performance of the experiment will then be demonstrated.

Task 9: Performance of Key Scavenging Characteristics

Sandia will measure the performance of key scavenging characteristics and assess the accuracy of the KIVA predictions and produce a scavenging development summary report.

Task 10: Sharing Alternator Development Data with CRADA

Sandia will share the alternator development data with CRADA partner Caterpillar, in turn receiving piston lubrication, cooling and sealing technology from CAT.

HYDROGEN SAFETY

Thick Film Hydrogen Sensor - Oak Ridge National Laboratory

Oak Ridge National Laboratory is developing a low-cost solid-state hydrogen sensor to support the long-term goals of the DOE Hydrogen Program to encourage acceptance and commercialization of renewable energy-based technologies. Development of efficient production, storage, and utilization technologies brings with it the need to detect and pinpoint hydrogen leaks to protect people and equipment. The solid-state hydrogen sensor, developed at ORNL, is potentially well-suited to meet cost and performance objectives for many of these applications. Under a Cooperative Research and Development Agreement (CRADA) and license agreement, ORNL is teaming with a private company, DCH Technology, Inc., to develop the sensor for specific market applications, related to the use of hydrogen as an energy vector. This CRADA will expire at the end of the year.

The plans for this year are directed toward the efficient transition of its sensor technology to industry. ORNL will have a small production run of hydrogen sensors made by a commercial hybrid circuit manufacturer, so that a large quantity of identical sensors are available for testing. ORNL will test these sensors to specifications provided by a large industrial end user of hydrogen sensors. By outsourcing the production batch, ORNL scientists can concentrate on further developing, optimizing, and understanding the fundamental materials and design issues rather than making large numbers of test pieces using bench-scale equipment. Based upon the outcome of these tests, ORNL will make materials and design improvements for later incorporation into the commercial sector. ORNL is also evaluating new designs that improve sensor performance and reliability, for which ORNL has applied for another U. S. Patent.

Task 1: Performance Testing

These tests will be conducted on ORNL-fabricated sensors and verified with commercially-produced sensors described in Task 2 below. The following tests will be performed:

- Repeatability. Characterize, understand, and improve (if necessary) sensor variation in day-to-day tests.
- Low-level response. For certain applications, it is desirable to trigger a detector response between 0 and 0.4% hydrogen in air. ORNL will examine the sensor mechanism to understand and potentially improve (speed up) the sensor response.

Thick Film Hydrogen Sensor
Oak Ridge National Laboratory (ORNL)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Performance Testing						
Conduct tests on sensors				◆		
Pilot production of Sensors and Testing						
Fabricate sensors commercially			◆			
Complete performance testing				◆		
Metallization, Design Modifications						
Complete design modifications					◆	

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- Continue characterizing the sensor cross sensitivity to other compounds that would likely be present in application scenarios.
- Continue long-term reliability and stability studies.

Task 2: Pilot production of Sensors and Testing

ORNL will produce small batch of sensors at commercial facility. ORNL realizes that the prototyping fabrication facility is limited in its ability to minimize variation between sensors. Also, sensor development has progressed to the point where ORNL is ready to evaluate commercially produced sensors. ORNL will have small batches of hydrogen sensors produced by one or more manufacturers. ORNL will test commercially produced sensors to automotive industry specifications. Sensor signal processing, design, and packaging will be performed by ORNL's CRADA partner.

Task 3: Materials Optimization for Reliability and Durability

In this task, ORNL will continue to explore the behavior of the Pd metallization at intermediate to high concentrations of hydrogen and evaluate modifications to the composition and structure of the metallization material to improve adhesion and stability without undue sacrifice of speed, sensitivity, and selectivity.

ORNL will produce small numbers of test samples in different conditions and examine them by scanning electron microscopy before and after hydrogen exposures to relate their structure to long-term performance. The main parameters to be explored are alloying of the metallization (particularly with Ag additions) and modified firing schedules. ORNL will also continue to explore novel design modifications such as H_2-permeable dielectric overcoats to protect the metallization from contamination and moisture as well as to provide mechanical support to improve adhesion at high H_2 concentrations. These overcoats will include porous co-fired ceramic films and polymer coatings.

Interfacial Stability of Thin Film Hydrogen Sensors – National Renewable Energy Laboratory

The real and perceived hazards of hydrogen fuel use, its production, and storage require extensive safety precautions and codes to be put in place before any serious movement can be made towards a hydrogen based energy future. Currently, commercial hydrogen detectors are not useful for widespread use, particularly in transportation, because they are too bulky, expensive, and dangerous. Recent work sponsored by the program has developed promising technologies for satisfying the future demands. Sensors which exhibit physical or optical changes when exposed to hydrogen have been fabricated, tested, and promise to provide inexpensive hydrogen detection. For example, there are thick film metallic sensors that exhibit a conductivity change when hydrogen adsorbs on the surface and is incorporated into the lattice. There are thin film sensors that are deposited as a part of a field-effect transistor, where a change in conductivity with hydrogen incorporation results in a response from the circuit. Finally, there are chemochromic sensors, where reaction of thin films with hydrogen gas results in an optical change that can be sensed by a probe beam of light. All of these sensors have the potential for degradation in their performance over time due either to mechanisms that are inherent in their construction, a result of their cyclic interaction with hydrogen, or contamination from impurities in the environments in which they will be used. NREL will study those issues in order to rank their importance to the various sensor concepts, will determine the relevant mechanisms, and orient the future work at the mitigation of these factors.

Task 1: Background Research

The initial effort will be research the materials used in the thin film sensors and learn as much about their chemical and physical properties as possible. NREL plans to carry out a comprehensive literature search and consult with experts in field.

Task 2: Laboratory Research

NREL will use analytical techniques to discover as much as possible about the failure mechanisms of thin film sensors constructed in prior work. In particular they will look at the issues of adhesion at the substrate/sensor interface, adhesion at the sensor/catalyst interface, and poisoning at the catalyst surface. Based upon the information obtained from these previous samples, they will design test coupons containing individual interfaces to study uncoupled reactions to cyclic exposure to hydrogen and impurity gases. Then, time and resources permitting, NREL will build interlayers designed to retard or eliminate the degradation mechanisms observed and test the validity of the models developed by this stage.

Interfacial Stability of Thin Film Hydrogen Sensors
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Analysis						
Rank the important mechanisms limiting the lifetime of the sensors				◆		

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Task 3: Analysis

The task team will collate all the background information, experimental results, and the most successful models of the interactions of the multi-layer films with hydrogen and impurity gases to rank order the degradation mechanisms at work in the sensors. This rank order can then be used to format the approach to increasing the lifetime of the sensors in the field and their resistance to impurities encountered in the environments in which they will have to work.

Dispersion of Hydrogen Clouds - University of Miami

A variety of topics have been addressed in the ongoing hydrogen safety research at the University of Miami. They include the following: Leakage from residential fuel lines, accidental combustion during hydrogen production, toxic chemicals used in hydrogen production, fuel gas cloud motion in residential structures, permeability of non-metallic pipes, flame visibility, flame arrestors, surface ignition, pipeline leakage, passive ventilation systems, leakage from compressed storage systems, cataloging of safety codes and standards, firewall testing, Humbolt State University Golf Carts, Savannah River Project Bus, odorant separation, safety codes and standards preparation, and rapid container filling.

Task 1: Simplification of the Hydrogen Risk Assessment Method to reduce the need for CFD Modeling

The method is used to determine the potential health and safety implications of a hydrogen release. The method allows the user to establish changes to venting in buildings and home refueling areas to minimize or eliminate any serious threats. It is the objective of this portion of the work to simplify the risk assessment method to eliminate or reduce the need for computer modeling in the method.

During the first five months of the work effort three potential worst-case partially enclosed geometries will be computer modeled to find the maximum differences between helium and hydrogen leakage in the enclosures. The geometries will be developed based on results from prior research and results from the models generated during the research.

During the second five months of the work effort the worst-case geometry identified by the computer modeling will be constructed and tested with helium and hydrogen leakage to verify the computer model predictions.

Dispersion of Hydrogen Clouds
University of Miami

Task Designation/ Milestone		2000				2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Simplification of H_2 Risk Assessment						
Model two potential worst-case accident	◆					
Model third potential worst-case accident		◆				
Construct and test worst-case				◆		
Develop H_2 risk assessment				◆		
H_2 Safety Information Dissemination						
Present safety material to NFPA for anticipated				◆		
Assist HyTEC				◆		
Assist with ISO/TC 197 WG6 and				◆		
Animate H_2 leakage into		◆				
Animate worst case				◆		

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During the last two months of the work effort guidelines will be developed for predicting hydrogen concentrations caused by leaking hydrogen from measured helium concentrations caused by leaking helium. This would allow risk assessment of a hydrogen leak scenario to be made by measuring the results of a controlled helium leak in the scenario.

Task 2: Hydrogen safety information dissemination to groups outside the hydrogen community

Methods for analyzing the risks produced by leaking hydrogen are not well known outside the hydrogen community. It is the objective of this portion of the work to increase the understanding of hydrogen risk assessment outside the hydrogen community.

Material will be presented for publication to the American Chemical Society and the National Fire Protection Association. Throughout the project, assistance to HyTEC (Hydrogen Technology Education Consortium) in developing a Clean Corridor Curriculum and Clean Corridor Implementation Workshops will be given as requested. Throughout the project, continued assistance in the writing of ISO publications will be rendered to ISO/TC 197/WG6 and ISO/TC 197/WG7.

During the first six months of the project the results of hydrogen leakage into a hallway, from previous research, will be animated. This will allow for better communication of the results to those outside the hydrogen community. Animation of the worst-case scenario data will be completed in the 12th month of the project and depictions will be included in the annual report.

Development of Codes and Standards from the Safe Use of Hydrogen – National Hydrogen Association (NHA)

Hydrogen plays a significant role in the world's energy economy, but this role is almost exclusively as a chemical - hydrogen is rarely used as a fuel. The use of hydrogen as a fuel in the utility and transportation sectors faces hurdles that need to be overcome in order to transition to a hydrogen energy economy. In addition to a lack of infrastructure to support the widespread distribution and use of hydrogen, there exists a persistent perception that hydrogen is unsafe. Widespread hydrogen use will require that safety be intrinsic to all processes and systems. To develop a hydrogen infrastructure that has the public's confidence in its safety and convenience, an industry consensus on safety issues is required. This includes the development of compatible standards and formats (e.g., the same couplings for dispensing the same form of fuel). Product certification protocols are also required. The development of codes and standards for the safe use of hydrogen is an essential aspect of the DOE Hydrogen Program.

The NHA is under contract with the U.S. Department of Energy, through the National Renewable Energy Laboratory, to identify and develop the standards necessary. Utilizing industry expertise and coordinating with Government and other official entities, this barrier to commercialization may be overcome, allowing siting of hydrogen components and systems on a world-wide basis.

Task 1: Development of Codes and Standards

The development of codes and standards for the safe use of hydrogen is an essential aspect of the DOE Hydrogen Program. The objective of this work is to continue the efforts already begun on the creation of draft international standards for safety, tanks, connectors, and refueling stations, as well as identify and begin work on additional needed standards to assure the safe use of hydrogen. NHA will continue active participation in NHA, ISO, IEA, and other relevant codes and standards arenas. New areas may include a broader role in fuel cell codes and standards.

Development of Codes and Standards for the Safe Use of Hydrogen
National Hydrogen Association (NHA)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Development of Codes and Standards						
Hold Codes and Standards meeting in Washington, DC			◆			
Mail proceedings from meeting				◆		
Hold Codes and Standards meeting in Washington, DC					◆	
Mail proceedings from workshop					◆	

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Integrated Micro-Machined Hydrogen Gas Sensors – Advanced Technology Materials, Inc.

Significant research and development efforts are currently underway to make the widespread use of hydrogen technically and economically feasible. These efforts are directed toward creating the basic building blocks of a hydrogen economy: production, storage, transport, and utilization. An underlying need of each of these building blocks is the ability to detect and quantify the amount of hydrogen gas present. This is not only required for health and safety reasons, but will be required as a means of monitoring hydrogen based processes. Hydrogen gas sensors that can quickly and reliably detect hydrogen over a wide range of oxygen and moisture concentrations are not currently available, and must be developed in order to facilitate the transition to a hydrogen based energy economy.

Phase I research efforts will be focused towards investigating sensor fabrication parameters, such as layer thickness and composition, and their effects on sensor performance; testing the hydrogen response of these sensors in wet/dry and oxygen-containing/oxygen-deficient atmospheres; and investigating the long-term stability of these materials and identification of limiting factors. Successful completion of this project will demonstrate the feasibility of using micro-hotplates in conjunction with palladium-coated metal-hydride films for sensing hydrogen in the environments required by a hydrogen based energy economy.

Task 1: Micro-hotplate Sensor Fabrication

The micro-hotplate device structures will continue to be fabricated via the MOSIS (Metal Oxide Semiconducting Implementation Service) foundry processes. MOSIS has MEMS-compatible fabrication runs scheduled approximately once every quarter, and the target is to submit three designs in the first seven months of the project. The first submission will be comprised of known and tested device structures in order to guarantee working samples for the subsequent tasks. The second submission will be comprised of several new layouts for testing purposes. New layouts will be created that are designed to investigate methods for minimizing device size, such as shrinking suspended surfaces and reducing the number of contact pads. The third submission will be comprised of proven device structures coupled with on board integrated electronics.

Integrated Micro-Machined Hydrogen Gas Sensors
Advanced Technology Materials Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Micro-hotplate Design and Fabrication						
Design and fabricate micro-hotplate				◆		
Functionalization						
Develop the functionalization process					◆	
Sensor Response						
Test sensor response					◆	
Sensor Lifetime Testing						
Test sensor lifetime					◆	

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Task 2: Micro-hotplate Functionalization

E-beam deposition processing will be the primary metallization deposition process in this project using an Airco Temescal multi-crucible, single gun, e-beam evaporation system. A statistically designed experimental plan will be constructed in order to screen multiple processing parameters and identify the most significant.

Task 3: Sensor Response Testing

An automated testing platform will be constructed that is capable of handling the gases mixtures of interest. The gases to be tested include the target gas of H_2, in addition to relevant backgrounds of nitrogen, air, and oxygen. Testing will be done in both wet and dry environments. In order to control the humidity, the gas test cell will be enclosed in a temperature controlled environment box. Measurement will be made at atmospheric pressure. The lower detection limits for hydrogen in these environments will also be probed. The gas test cell will be completed in the second month and response testing will begin in the third month of this program.

Task 4: Sensor Lifetime Testing

An automated lifetime testing apparatus will be constructed that will allow multiple sensor chips to be run continuously for time periods of a month or more in air. The responsiveness of these sensors will be tested in the automated response-testing platform before and after these continuous lifetime tests. Both the lifetime of the heater element and the reactive layer will be monitored.

3.2 Technology Validation

This section describes the projects that are being considered as key hydrogen implementation components. They include ongoing studies of hydrogen transportation systems including hydrogen clean corridor efforts, and a series of feasibility studies awarded as the first phase of projects addressing various hydrogen-related business opportunities. Most of these projects are team efforts involving a prime contractor and at least one subcontractor. The projects are identified by the identity of the prime contractor. Technology Validation Tasks are listed in Table 3.5.

Table 3.5
Technology Validation

Goal: Support industry in the development and demonstration of hydrogen systems in the utility and transportation sectors

Category	Project	Researcher
Renewable Hydrogen Systems	Hydrogen Production Through Electrolysis	Proton Energy Systems
Hydrogen Infrastructure	Advanced Chemical Hydride Hydrogen Generation/ Storage System for PEM Fuel Cell Vehicles	Thermo Power Corporation
	An Integrated PV / Electrolysis / Metal Hydride Hydrogen Generation and Storage System for Scooter Applications	Energy Conversion Devices, Inc.
	Filling up With Hydrogen 2000	Stuart Energy Systems
	Hydrogen/Natural Gas Blends	NRG
	Integrated H_2 Fuel Infrastructure Research and Technology Development	National Renewable Energy Laboratory
Remote Power	Alaska PEM Fuel Cell Validation Project	Sandia National Laboratories
	Hydrogen-Based Utility Energy Storage System	SRT Group

RENEWABLE HYDROGEN SYSTEMS

Hydrogen Production Through Electrolysis – Proton Energy Systems, Inc.

Products based on Proton Exchange Membrane (PEM) technology offer a unique solution to today's energy conversion storage needs. PEM products have undergone continual development since the late 1950's for many diverse applications. Rooted in rigorous aerospace applications, this technology is now "breaking away" to provide commercial solutions to common power, energy, and industrial gas feedstock problems. Important developments in PEM electrolyzers and various energy conversion devices (e.g. engines and fuel cells) can now be combined to form the basis for a revolutionary energy storage system that provides a much needed link to renewable resources, and offers a credible alternative for off-grid power applications.

This technology operates by converting electrical energy into chemical energy in the form of hydrogen as part of a water electrolysis process when excess power is available. When the primary source of power is unavailable, chemical energy is converted into electrical energy through an external combustion heat engine.

The goal of this project was to demonstrate a pathway to a sustainable energy system using a PEM hydrogen generator coupled to a SunDish™ concentrating solar thermal system. The SunDish system generates electricity during daytime operation by concentrating solar energy into a Stirling external heat engine. The hydrogen generator generates and stores hydrogen during daytime operation and feeds the hydrogen into the Stirling engine to generate electricity at night or on cloudy days. The system has been installed at the Ocotillo Power Plant owned by Arizona Public Service in Tempe, Arizona since May of 1999. The objective was to store 200 Kilowatts (kW) of power in the form of hydrogen and use that stored gas to run the engine on the SunDish system. In addition, a business plan was to be created to describe in detail, hydrogen energy storage products as they relate to off-grid or select on-grid applications.

Improved electrical energy storage products that enable large amounts of energy to be stored cleanly, simply and efficiently can have a profound impact on the delivery of energy services. Previous technology relied on conventional batteries which have limitations on duration of storage, cycle life,

Hydrogen Production Through Electrolysis
Proton Energy Systems, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Reduction of Hydrogen Generation Costs						
Introduce improved cell stack component modifications					◆	
Complete design of low cost generator components					◆	
Design and Testing						
Design and test of generator circuit card					◆	
Construction of HOGEN Electrolyzer						
Implement membrane and catalyst improvements					◆	
Implement flow field improvements					◆	

Figure 2000 Begins October 1, 1999

depth of discharge, and self-discharge, and have entailed the use of toxic or hazardous materials such as lead and sulfuric acid. Storage of electrical energy as hydrogen has the potential to provide such a capability at a far lower initial and overall cost than batteries without these performance and environmental restrictions.

Work in Phase II will focus on demonstrating PROTON's UNIGEN® regenerative fuel cell technology. This technology, once matured, will enable PROTON® electrolyzer hardware to work in both directions—as an electrolyzer making hydrogen and as a fuel cell converting that hydrogen back into electricity.

The tasks below will describe an approach for Phase II that de-emphasizes the full-scale development and testing of complete systems discussed in the original proposal and focuses needed resources on an intensive effort aimed at cost reducing the electrolysis portion of the UNIGEN. The original Phase II had quite a bit of effort focused on cost reduction and the current plan is to carry it forward into the system controls and power interface arenas as well as expanding it to encompass more facets of the cell stack design.

Task 1: Reduction of Hydrogen Generation Costs

PROTON proposes to reduce the cost of our hydrogen generator family by 50% in the next two years and show evidence of further dramatic reductions in the years beyond. We will do this by focusing cost reduction efforts on three key elements of the electrolyzer, the electrolysis cell stack, the power conditioning and renewables interface, and the electrical controls and software. We will complete the design of low cost components for the hydrogen generator and introduce improved cell stack component support modifications.

Task 2: Implementation of Cost Reductions

PROTON will implement interim improvements in membrane, catalyst and flow fields on our smaller (HOGEN® 40) electrolyzer first and expand those improvements to the larger electrolyzer towards the end of the program.

Task 3: Design and Testing

PROTON will complete the design and testing of a reduced-cost generator circuit card.

Task 4: Construction of HOGEN Electrolyzer

PROTON proposes to build a HOGEN 40 within the first twelve months of the program that implements all or most of the improvements undertaken. In addition, we will subsequently modify one or more HOGEN 300/380 systems by the end of Phase II to prove out the cost reductions in the large sized generator.

HYDROGEN INFRASTRUCTURE

Advanced Chemical Hydride Hydrogen Generation/Storage System for PEM Fuel Cell Vehicles ─ Thermo Power Corporation

The objective of this program is to develop a prototype, 50 kW electric power equivalent hydrogen supply system utilizing an innovative chemical hydride/organic slurry technology. The system goals are to construct a hydrogen storage system with a gravimetric power density of greater than 3355 Whr/kg and a volumetric power density of greater than 929 Whr/liter

Because of the inherent advantages of high efficiency, environmental acceptability, and high modularity, fuel cells are potentially attractive power supplies. Worldwide concerns over clean environments have revitalized research efforts on developing fuel cell vehicles (FCV). As a result of intensive research efforts, most of the subsystem technology for FCV's are currently well established. These include: high power density PEM fuel cells, control systems, thermal management technology, and secondary power sources for hybrid operation. For mobile applications, however, supply of hydrogen or fuel for fuel cell operation poses a significant logistic problem.

Currently, various technologies have been considered to provide hydrogen for FCV's. These technologies can be conveniently classified into two categories: (1) onboard fuel processing wherein liquid fuel stored on the vehicle undergoes reformation and subsequent processing to produce hydrogen; and (2) onboard storage of pure hydrogen provided by stationary fuel processing facilities. Onboard liquid hydrocarbon reforming provides an attractive way to supply hydrogen at a high system power density. In high temperature fuel cells, such as solid oxide fuel cells, low molecular weight hydrocarbons may be used directly via direct internal reforming. However, these types of fuel cells are not suitable for fuel cell vehicles, since they may require frequent on/off cycling. Although there has been limited success in direct methanol powered PEM fuel cell technology, the fuel crossover and CO poisoning still pose significant problems, and long-term performance is yet to be demonstrated.

Advanced Chemical Hydride Hydrogen Generation/Storage System for PEM Fuel Cell Vehicles
Thermo Power Corporation

	2000					2001	
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2
Evaluate Performance of Prototype System							
Complete shakedown testing	◆						
Complete performance testing		◆					
Integrate H2 Generator with Simulated Fuel Cell							
Modify design of subcomponents		◆					
Complete shakedown tests			◆				
System Testing and Peformance Evaluation							
Complete performance evaluations				◆			
Deliver generator system to ANL				◆			

Figure 2000 Begins October 1, 1999

To supply high purity hydrogen for FCV operation, Thermo Power Corporation, Advanced Technologies Group, is evaluating a metal hydride/organic slurry to store and carry hydrogen. At the point of use, high purity hydrogen will be produced by reacting the metal hydride/organic slurry with water. The spent hydride can be relatively easily collected at the pumping station and returned to a centralized regeneration plant. In its other project, noted above, Thermo Power Corporation is researching the regeneration process steps required to return the metal hydroxide waste back to metal hydride. Regeneration with renewable sources such as biomass, natural gas, or coal are being evaluated. The fluid-like nature of the spent hydride/organic slurry provides a unique opportunity for pumping, transporting, and storing the slurry. The final product of the program will be a user-friendly and relatively high energy storage density hydrogen supply system for fuel cell operation.

Task 6: Evaluate Performance of the Prototype System

The purpose of this task is to evaluate the performance of the prototype mobile hydrogen generator. The system will be evaluated over a range of hydrogen flow rates up to 3 kg/hr.

Task 7: Integrate the Hydrogen Supply System into Operating Conditions of Simulated Fuel Cell Power Source

The purpose of this task is to improve the Prototype System and to simulate the hydrogen generation for a simulated fuel cell automotive power supply.

Task 8: Complete System Testing and Performance Evaluation

The objective of this task is to demonstrate the performance of the final version of the hydrogen supply system. The system will be delivered to Argonne National Laboratory ready to supply a fuel cell stack.

An Integrated PV / Electrolysis / Metal Hydride Hydrogen Generation and Storage System for Scooter Applications - Energy Conversion Devices, Inc. (ECD)

The overall objective of this twelve month phase II work is to develop an Integrated PV / Electrolysis / Metal Hydride based hydrogen generation and storage system for scooter applications. The objective will be met by the following tasks.

Task 1: Detailed Market Analysis for Hydrogen Scooters

A detailed market study was presented at the April 1999 DOE review meeting. This is an on-going task and will continue in collaboration with Piaggio with particular reference to developing countries.

Task 2: Metal Hydride Storage System (MHSS) Development

Subtask. 2.1: Preliminary alloy selection
Alloy selection will be based on hydrogen storage properties and their tolerance to moisture laden electrolytic hydrogen.

Subtask 2.2: Mathematical modeling and simulation of MHSS
Computer simulation of hydride storage containers will be studied to optimize the system design and performance.

Subtask 2.3: Alloy Compaction
Several different packaging methods will be evaluated to enhance heat and mass transfer.

An Integrated PV / Electrolysis / Metal Hydride Hydrogen Generation and Storage System for Scooter Applications - Energy Conversion Devices, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Design metal hydride storage container		◆				
Test metal hydride storage system			◆			
Component Integration						
Specify and design PV module						
Integrate electrolyzer with PV	◆					
Integrate electrolyzer with MHSS			◆			
Electrolyzer R&D						
Conduct R&D		◆				
Hydrogen Scooter						
Convert scooter to run on hydrogen			◆			

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Subtask 2.4: Metal Hydride Storage Container design
Container design will be optimized taking into account the overall heat and mass transfer, safety, weight and volume considerations.

Subtask 2.5: Metal Hydride Storage System testing
The storage system thus designed will be tested for overall performance including storage capacity, and hydrogen delivery rate under different pressure and temperature conditions.

Task 3: Component Integration

Subtask 3.1: PV module specification and design
United Solar Systems Corp. (USSC) will design a PV module according to Stuart Energy Systems' (SES) specifications for providing power to the alkaline electrolyzer.

Subtask 3.2: Integrate Electrolyzer with PV
SES will integrate the PV module with the electrolyzer, test it and deliver to ECD.

Subtask 3.3: Integrate Electrolyzer with MHSS
The control and instrumentation issues will be addressed while integrating the electrolyzer to the MHSS.

Task 4: Electrolyzer R&D

SES will develop a higher-pressure electrolyzer according to their statement of work.

Task 5: Hydrogen Scooter

Piaggio will develop and build a hydrogen –ICE, convert a scooter to run on hydrogen, and deliver the scooter to ECD. ECD and Piaggio will perform further system integration. This task is expected to extend to phase III.

Filling Up with Hydrogen 2000 - Stuart Energy Systems

Under the program "Filling Up With Hydrogen 2000" hydrogen vehicle re-fueling systems, called fuel appliances will be developed in a prototype development program which builds on Stuart's electrolysis technology. The fuel appliance combines the components needed to convert water and electricity to high-pressure hydrogen gas. The system consists of an electrolyzer, compressor and refueling dispenser packaged in one or more easy to deploy units. The fuel appliance systems can be built to suit a wide range of hydrogen supply capacities, from the size needed to fuel a single vehicle over night, a unit Stuart calls a Personal Fuel Appliance (PFA) to larger service stations, named Packaged Hydrogen Supply Appliances, which can support many vehicles, including large fleets of buses.

Task 1: Personal Fuel Appliance (PFA)

The first working model, P1 Model 10, producing 20 SCFH, has been built and successfully tested. The unit has been demonstrated to representatives from Daimler-Chrysler, Ford and General Motors. Based on this unit a major North American automaker has agreed to test and evaluate the P1 Model 25 prototype, which will produce up to 50 SCFH to amximum pressure of 3600 psig. Construction of the P1 Model 25 has started and is expected to be completed in Q4 1999. Testing is expected to begin Q1 2000 with release for outside evaluation before the end of Q1 2000.

Task 2: Packaged Hydrogen Supply Systems

Assembly of P3-1A was completed in Q2 1999, with the start of factory testing at the end of Q2 1999. P3-1A, a 1500 SCFH unit reaching a maximum pressure of 4000 psig, will be deployed at SunLine Transit at their bus garage in 1000 Palms CA where it will be used to fuel a fleet of hydrogen and Hythane vehicles. Delivery to California is expected when buses arrive in Q2 2000. In the meantime P3-1A will be run at Stuart's test facility. The design of the P3-1B has been completed and start of process testing is expected by Q4 1999. Unlike P3-1A which uses Stuart's CST Multi-stack Electrolyzer technology, P3-1B will use a train of CST Single Stack Electrolyzers. Two units of 400 SCFH will be built in Q1 2000, and will be deployed in hydrogen vehicle demonstrations expected to start in Q2 2000. Design of the P3-10 feuler, able to support a fleet of 10 fuel cell buses, has been taken to the concept stage and will be pursued to the design and costing stage in Q2 2000,with deployment and testing pending identification of a suitable deployment site. Development of the P4 technology was launched with testing a new pressure control system in a large single stack cell, similar to that used in the PFA Model 10 single vehicle refueler. Design of a P4 fuel appliance is planned to begin in Q2 2000 with a unit ready to deploy by Q4 2000.

Stuart Hydrogen Infrastructure Project – Stuart Energy Corporation

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Personal Fuel Appliance						
Assembly of P1 model 25 prototype	◆					
Releas of P1 Model 25 for evaluation by industry			◆			
Packaged Hydrogen Supply Appliance						
Deliver P5-1A to Sunline Transit			◆			
Finish assembly of P3-1B process	◆					
Build two P3-1B appliances			◆			
Design and cost P3-10 appliance				◆		
Build P4 appliance					◆	

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Hydrogen/ Natural Gas Blends – NRG

INPUT NOT RECEIVED

Integrated Hydrogen Fuel Infrastructure Research and Technology Development - National Renewable Energy Laboratory

This project is a comprehensive effort to integrate federal and state hydrogen fuel infrastructure research and technology development. This project will address hydrogen as a fuel for fuel cell vehicles, as a fuel for subsonic aircraft, and as an energy storage medium in renewable hybrid electricity generation systems. For vehicular applications, the project will integrate fuel distribution, storage, and dispensing requirements; safety requirements and analyses; performance data collection and evaluation; codes and standards requirements; and insurance and liability issues related to hydrogen fuel infrastructure and hydrogen vehicle development. For aircraft applications, the project will assess hydrogen fuel infrastructure requirements for commercial aircraft in regular service. For stationary electricity generation, the project will test wind/photovoltaic and electrolyzer/fuel cell hybrid systems using hydrogen for energy storage. The project will continue providing technical support to the HTAP, coordinating hydrogen projects and programs with other government agencies, and developing a comprehensive approach to codes and standards development for hydrogen applications.

Task 1: Hydrogen Fuel Infrastructure Research and Technology Development for Buses and Automobiles

NREL will continue to assist DOE in coordinating hydrogen fuel infrastructure research and technology development for automobiles and buses, particularly in transit applications, with other federal agencies and with state and local entities, especially in California.

Integrated Hydrogen Fuel Infrastructure Research and Technology Development
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
H2 Fuel Infrastructure Research and Development						
Conduct H2 fuel infrastructure workshop		◆				
Develop H2 fuel infrastructure blueprint					◆	
Draft data acquisition protocol				◆		
Conduct DOE/CFCP workshop on fuel choice			◆			
Hydrogen Fueling Infrastructure for Aircraft						
Draft MOU to submit to EERE		◆				
Hybrid Hydrogen Fuel Cell System Development						
Finalize NASA/DOE agreement to transfer fuel cell			◆			
Conduct initial system check-out tests					◆	
Hydrogen Safety						
Draft sourcebook for building and fire code officials				◆		

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Subtask 1.1: Hydrogen Fuel Infrastructure Development Blueprint
NREL will prepare a multi-year blueprint for hydrogen fuel infrastructure research and technology development. The objective of the blueprint is to prepare a plan to field-test concepts of hydrogen fuel infrastructure development proposed by DOE Hydrogen Program. These concepts include small-scale hydrogen generation and dispensing to serve the initial introduction of fuel cell and other hydrogen-fueled vehicles. As part of the plan, hydrogen fuel infrastructure based on small-scale, on-site electrolyzers and small-scale natural gas reformers will be developed and tested in conjunction with vehicle development.

Subtask 1.2: Technical Coordination of California Hydrogen Bus Technology Development
NREL will continue to coordinate technology development and data acquisition for the three hydrogen bus development projects funded by FTA/DOT and the CEC in California through the California Hydrogen Bus Coordination Committee. NREL will work with the technical staff of the three bus projects as required to advance the state of technology in platforms, propulsion systems, and fuel systems and fueling infrastructure. NREL will help develop common data acquisition procedures and protocols with the three transit agencies. The procedures and protocols will be based to the extent feasible on those developed under the DOE Alternative Fuel Transit Bus Evaluation Program. Data and information essential for codes and standards development and for insurance and liability matters will also be collected.

Subtask 1.3: Programmatic Coordination with California Fuel Cell Partnership
NREL will work with CARB, CEC, and the California Hydrogen Bus Coordination Committee to integrate on-going and planned hydrogen bus projects in California with the California Fuel Cell Partnership (CFCP). Key activities include coordination on fuel choice and fuel infrastructure development, location and testing of fuel cell buses, codes and standards for safety and insurance, data acquisition and dissemination, public information and education.

Task 2: Hydrogen Fueling Infrastructure for Subsonic Commercial Aircraft

Subtask 2.1: Memorandum of Understanding with NASA
NREL will assist DOE in the development and adoption of a memorandum of understanding (MOU) for cooperative and collaborative research and development of hydrogen technologies. Task agreements under the MOU will address specific R&D projects on hydrogen-fueled subsonic aircraft and fueling infrastructure.

Subtask 2.2: Scenario Development and Assessment of Hydrogen Fueled Aircraft
NREL will develop preliminary scenarios for subsonic hydrogen-fueled aircraft in commercial service with NASA and with the aircraft, airline, and hydrogen industries. These scenarios will be evaluated by a peer review committee selected by DOE and NASA. One or more of the scenarios will be selected for detailed assessment in FY2001. The intent of the scenario development and assessment is to prepare for a demonstration of a hydrogen-fueled aircraft in FY 2002 under joint funding by DOE and NASA.

Task 3: Hybrid Renewable Energy-Hydrogen Fuel Cell System Development

NREL will work with NASA and the DOE Photovoltaic and Wind Energy programs to assess system integration issues for linking fuel cells and electrolyzers to wind turbines and PV modules. NREL will obtain NASA's PV-electrolyzer-fuel cell system now at Edwards Air Force Base and install the system at the Hybrid Power Test Bed at NREL's National Wind Technology Center (NWTC). The NASA system will be tested with selected wind turbines at the NWTC and with PV modules provided by NREL's PV test facility to assess system integration issues, including the technical and economic viability of hydrogen energy storage to provide dispatchable energy from wind and PV systems. In the future, the test bed could be used to conduct comparative evaluations of other energy storage options, e.g., advanced batteries, flywheels, that could compete with hydrogen fuel cell-electrolyzer systems.

Task 4: Hydrogen Safety

NREL will continue to assist DOE develop codes and standards for hydrogen applications.

Subtask 4.1: Sourcebook Adaptation for Building and Fire Code Officials
NREL will adapt version 1.0 of the *Sourcebook for Hydrogen Applications* to address the specific concerns of building and fire code officials. This work will be co-funded by Canada Natural Resources through the Hydrogen Research Institute at the University of Quebec. The *Sourcebook* will be tailored in content and format so that it can be presented to selected organizations of building and fire code officials. NREL will work with the NHA and other constituent groups to establish the necessary interactions with officials of these selected organizations so that the tailored version of the *Sourcebook* complements the normal process the code officials follow to adopt new information and requirements into building and fire codes.

Subtask 4.2: Comprehensive Hydrogen Safety Code Development
NREL will work with DOE to evaluate options on how to develop a code for hydrogen use that is adopted and promulgated by International Code Council (ICC). Options on tactics to attain this goal may include a separate chapter on hydrogen instead of modifications of existing codes to address hydrogen issues. NREL will also assist Program interactions with the BOCA, NFPA, and other entities within and outside of the ICC and help to facilitate and manage inputs from NHA, the California work (Task 2.1), and elsewhere into the ICC process. An annual status report on hydrogen codes and standards to be delivered at NHA or HTAP each spring.

REMOTE POWER

Alaska PEM Fuel Cell Validation Project – Sandia National Laboratories

Sandia National Laboratories is providing technical program management in support of a development and deployment remote area power program for Alaskan applications. Fuel utilization in remote Alaskan villages is far from optimal. Electrical power is generally produced from diesel generator sets resulting in a multitude of problems for example: this power is very expensive, unreliable, and results in air, ground and water pollution. The waste heat from these generator sets is often used to heat a large nearby building like a school, however, the individual dwelling owner does not directly benefit from this waste heat which frequently represents 60% of the overall energy requirements. This Alaskan Proton Exchange Membrane Fuel Cell (PEMFC) Program provides an opportunity to adapt developing PEMFC technologies to provide an integrated solution for improved fuel utilization for the arctic Alaskan villages.

One of the goals of this program is to provide PEMFC systems producing 3-5 kW of grid quality power engineered for remote applications in the arctic climate of Alaska. These PEMFC systems will be engineered to maximize fuel utilization addressing the dwellings entire energy needs, including all electrical, space and water heating needs. This will significantly reduce the overall energy consumption in Alaskan remote villages and increase electrical system reliability. As a transition strategy these first PEMFC systems are to be operated on hydrogen from reformulated diesel fuel. This will position the Alaskan villages to eventually replace the dependence on diesel fuel and shift to some other form of energy, for example, renewables.

There were three distinctly separate projects associated with phase I of this program. In phase II there are two projects. Each project is performed by a team of industrial partners in collaboration with Sandia National Laboratories, The Alaskan State Energy Office, and The University of Alaska at Fairbanks (UAF). This program is designed to be executed in three phases. These phases, milestones and progress to date are listed below.

Task 1: Diesel Reformer/ PEMFC System

A diesel reformer / PEMFC system must be delivered and have the capability of hands off operation with all the suitable control systems and power conditioning equipment in place to produce grid quality power. This unit must be at least a post laboratory, pre-pre-prototype system. This system must be delivered, installed and made operational in the Sandia specified laboratory environment between September 30, 1999 and December 31, 1999.

Integrated Hydrogen Fuel Infrastructure Research and Technology Development
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Diesel Reformer/ PEMFC System						
Deliver pre-prototype automated PEMFC system			◆			
Complete pre-prototype qualification by UAF				◆		
Begin field testing				◆		

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A diesel reformer / PEMFC / Power conditioning system shall have the capability to provide power for a single structure (i.e. private residence or small commercial building). The Reformer / PEMFC / Power conditioning system will be part of a hybrid system using an energy storage system to supply the peaking needs of the application of choice. The size for this system will produce 3 - 5 kW base load. This system must be at least a pre-commercial prototype. The energy storage system will be designed to handle the peaking demand as determined by the end use. This system must be delivered, installed and made operational in the TBD Alaskan remote application between September 30, 2000 and December 31, 2000.

The industrial teams each bring a unique technology to this program which will be promoted and evaluated for suitability in the Alaskan Arctic climate. These teams consist of:

Northwest Power Systems is providing a steam reformation and systems integration of their reformer and a 3 kW PEMFC. Northwest Power Systems, Sandia National Laboratories and UAF are evaluating a number of stacks from different vendors for suitability for this project.

Teledyne Brown Engineering (TBE) has teamed with Schatz Energy Research Center (SERC) to deliver an integrated system. TBE will purchase a reformer from Northwest Power Systems for integration with SERC's pure hydrogen PEMFC stack. TBE is providing systems integration and technical team program management.

As noted above both activities are held to the same three program phases with the same deliverables. At the end of the program SNL will have designed and evaluated each component and system for use as distributed power generation in Alaska's arctic climate. Indeed, a total of 6 to 7 PEMFC stacks will be evaluated with 1 to 2 chosen for final integration in phase III of this program. In collaboration with other DOE hydrogen activities SNL and UAF are evaluating a total of 4 to 5 different reformation technologies for suitability in Alaska.

SNL will seek an additional industrial partner to deploy a PEMFC / autothermal reformation system. This new project will be aligned with the currently planned phase III program and held to the same deliverables and milestones. This industrial partner will be selected through a competitive bid process and as of the writing of this document remains to be determined (TBD).

Hydrogen-Based Utility Energy Storage System – SRT Group

The SRT team is now entering Phase II of an effort developing a novel means for storing energy from electricity that is supplied from a renewable source. This approach is also applicable to electrical energy storage needs in other scenarios, such as distributed power, and is capable of cost effective load management without needing standby or peak generation facilities.

The system is based on using electricity generated during periods of low demand to electrolyze hydrobromic acid (HBr) in an electrolyzer into hydrogen (H_2) and Bromine (Br_2). During high demand periods the hydrogen and bromine are recombined in the same unit, acting as a fuel cell, to regenerate the electricity. By careful scheduling of charging and discharging phases, energy storage by the system can obviate the need for expensive peaking generation units. As the system does not emit any waste products such as CO_2, wastewater, or solid waste, permitting issues are eased, and the system can be situated near the load, saving the need to expand generating, transmission, and switching capacity solely to meet peak generating requirements.

Team member National Power PLC is currently working on a regenerative HBr/H_2Br_2 fuel cell that has been designed for low cost manufacturability. This cell is expected to cost $350 per kilowatt in production quantities.

The program plan for Phases I, II and III will move the project forward with an ambitious schedule to deliver the ultimate goal of a meaningful demonstration in Alaska of the SRT team energy storage/hydrogen production concept. In Phase I of the project, a 50 kW HBr electrolysis system provided by National Power (NP) was built and will shortly be installed into a test stand for the purpose of obtaining necessary data for a regenerative electrolyzer or fuel cell. This will allow checkout of the system, and will allow NP to proceed with the construction of a prototype100 kW reversible system. In Phase II the 50 kW electrolysis system will be replaced with the 100 kW prototype reversible fuel cell system, and the unit will be tested. The lessons learned from Phase II will be utilized in Phase III to refine the preliminary system design and fabricate a production system capable of producing and using HBr from bromine and hydrogen to store and produce energy in the form of electricity. The system will be installed in Alaska in a building on a site that will be prepared as part of the effort. The system will be fully instrumented and tested to determine its response to process variables and these will be utilized to determine process economics for the system.

Hydrogen-Based Utility Energy Storage System
SRT Group

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
50 kW Electrolysis Prototype System						
Complete testing				◆		
100 kW Regenerative Cell Demo						
Design 100 kW HBr regenerative system				◆		
Fabricate 100 kW system				◆		
Modify 100 kW electrode				◆		
Deliver stack for testing				◆		
Bench test and evaluate system						

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Task 1: 50 kW Prototype Electrolysis System

In this task the overall objective was to perform a preliminary design for the major components required for the energy storage system. In addition, a system design will be undertaken. Specifications for the system will be determined and reviewed. The conceptual system designs produced by SRT will be reviewed and evaluated for consistency, safety and the ability to manufacture parts from the drawings. During this task, a design effort for the 50 kW test stand was also made.

Subtask 1.1: 50 kW Electrode Modification/Stack Manufacture
Modifications to the electrode configuration and composition of the National Power electrolysis cell to accommodate the HBr couple were made. Several trial configurations and materials were tested to ensure compatibility and utility. The 50 kW electrolysis system was manufactured.

Subtask 1.2: Hydrogen Catalyst Modifications
The hydrogen catalyst was modified to be compatible with reversible service. Several candidate catalyst formulations and configurations were tested to determine which is the most useful. The one picked has been tested to determine the projected lifetime and has been applied to the membrane for use in the 50 kW prototype. After testing, modifications to the catalyst will be made if required and the catalyst will be applied to the 100 kW prototype reversible cell stack system.

Subtask 1.3: Hydrogen Bulk Diffusion and Seal Diffusion Measurements
In this task, the rate of diffusion of hydrogen through the cell materials and cell seals was measured and minimized through the use of manufacturing techniques to hold size tolerances to a standard and minimize thin areas. In addition the seal diffusion rates were minimized or controlled by the modification of the seal design.

Subtask 1.4: Bench Test and Evaluate 50 kW system
The 50 kW test stand will be constructed and the 50 kW electrolyzer will be placed into service and tested. Testing will involve determination of projected electrode lifetimes, achievable current density and optimum operating parameters.

Task 2: 100 kW Prototype Reversible System

In Task 2 the 50 kW electrolysis only prototype system will be replaced and updated with a 100 kW prototype reversible system. This system will be capable of storing energy, but will be for development only. In this prototype system, the major items requiring development will be the controls and electrode materials.

Subtask 2.1: Design and Fabricate 100 kW HBr Regenerative System
The prototype 100 kW reversible cell will be designed and fabricated. A Prototype 100 kW regenerative system test stand will also be designed and fabricated. The system will employ controls, sensors, power conditioning and ancillary equipment similar to but smaller than the Phase III unit.

Subtask 2.2: 100kW Electrode Modifications
The electrode size and configuration will be modified based on data gathered in task 1.2. As the area of each cell will be larger, the configuration will need to be redesigned. In addition, attachment points and manufacturing methods for production will need to be established.

Subtask 2.3: Bench Test and Evaluate 100 kW system
The 100 kW reversible electrolyzer will be tested on the test stand to determine performance and optimum operational requirements. Data gathered from this testing will be used in Phase III to design the 350kW reversible production ready unit for delivery to Alaska.

3.3 Analysis and Technology Transfer

This element includes projects in the areas of analysis (process, systems, and integration) and in the transfer of technology both domestically and internationally. Projects are being undertaken at universities, national laboratories, and in industry.

The analysis area is made up of projects involving analysis of technology development and validation processes, analysis of integrated systems, and integrated analysis of major components of the overall program. The systems analysis area consist of environmental, economic, and market analyses of potential hydrogen energy systems, their subcomponents, and the supporting infrastructure, as shown in Table 3.6. The products of these analytical studies will be used by the DOE Program Manager to establish program priorities for R&D as well as for near-, mid-, and long-term component, subsystem, and system validations.

Table 3.6
Analysis Projects

Goals:

- **Ensure that Federal R&D investments in hydrogen production, storage, distribution, and end-use technologies will provide the maximum value added to national strategic goals including global greenhouse emission mitigation;**
- **Identify and evaluate key market segments and market entry conditions for hydrogen utilization in transportation and in electricity generation at distributed and remote locations; and**
- **Develop and apply metrics to measure the Program's contribution to attaining national strategic energy goals and market share in key market segments.**

Category	Project	Research
Analysis Activities	Process Analysis of Hydrogen Research Activities	National Renewable Energy Laboratory
	Distributed Hydrogen Fueling Systems Analysis	Directed Technologies, Inc.
	Hydrogen Energy System Studies	Princeton University
	Strategic Response to Scenario Planning	National Renewable Energy Laboratory

ANALYSIS ACTIVITIES

Process Analysis of Hydrogen Research Activities - National Renewable Energy Laboratory

Process analysis provides direction, focus, and support to the development and introduction of hydrogen through evaluation of the technical, economic, and environmental aspects of hydrogen production technologies. Such analyses allow NREL to determine the prospects that a process will be economically competitive with conventional systems, and to identify opportunities that will result in cost reductions. Additionally, the environmental benefits of renewable technologies can be quantified and integrated with the economics of the process.

The technical, economic, and environmental aspects of technologies being researched in the Hydrogen Program are evaluated. Broadly speaking, two analysis methods are used to effect this work. First, technoeconomic analyses (TEA) are performed to determine the potential economic viability of a research process. Second, life cycle analysis (LCA) is used to evaluate the environmental benefits and drawbacks of the process.

The second analysis tool, LCA, is an analytic method for identifying, evaluating, and minimizing the environmental impacts of emissions and resource depletion associated with a specific process. When such an assessment is performed in conjunction with a technoeconomic feasibility study, the total economic and environmental benefits and drawbacks of a process can be quantified. Material and energy balances are used to quantify the emissions, resource depletion, and energy consumption of all processes required to make the process of interest operate, including raw material extraction, processing, and final disposal

Process Analysis of Hydrogen Research Activities
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Update of the Cost of Hydrogen						
Updated cost of PEC hydrogen production		◆				
Assessment of Wind Energy Coupled with Fuel Cell						
Assess feasibility of using a fuel cell for wind energy			◆			
Life Cycle Assessment						
Assess life cycle of renewable hydrogen producing system			◆			
Update of Cost from Hydrogen from Biomass						
Report on the cost of hydrogen from biomass				◆		
Analysis of Production of H2 from SER & ITM Reactors						
Analyze production of H2 via the ITM and SER reactors				◆		
Evaluation of Photobiological H2 Production						
Report on the cost of H2 production via algal systems					◆	
Comparison of On-board Hydrogen Storage						
Report on literature review of on-board H2 storage		◆				

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of products and by-products. The results of this inventory are then used to evaluate the environmental impacts of the process so that efforts can be focused on mitigating these effects.

Task 1: Analysis of New Projects, Funded or Proposed

As new projects are proposed for funding by the Hydrogen Program, they will be analyzed to determine their potential for economic viability. These analyses will likely be limited to cost boundary, and will include many alternative cases to take into account possible research advances. Additionally, analysis support will be provided to those organizations who are selected for funding under current and future solicitations. Work on this activity will be performed at the request of Hydrogen program management, as new project ideas are proposed.

Task 2: Update of the Cost of Hydrogen from a Photoelectrochemical Hydrogen System

New information on the cost of capital for a photoelectrochemical hydrogen production system will be incorporated into the analysis conducted in FY 1998 to update the projected cost of hydrogen. Additionally, a detailed Monte Carlo sensitivity analysis will be conducted to determine which parameters most greatly influence the results.

Task 3: Assessment of Wind Energy Coupled with a Reversible Hydrogen Fuel Cell
An analysis will be performed on the production of electricity from wind turbines coupled with energy storage in a reversible fuel cell. The wind turbines will be assumed to be located in the North-Central region of the U.S., while energy demand will be elsewhere. A reversible fuel cell will be used to produce hydrogen, which will be converted back into electricity during periods of high demand, and thus higher price opportunities. Different ratios of production to demand will be studied. It is possible that a subcontract mechanism will be used to obtain the right combination of expertise in the electricity markets and hydrogen technologies. Results will show the technical and economic feasibility of this concept.

Task 4: Life Cycle Assessment

Life cycle assessment is used to quantify the environmental benefits and drawbacks of a system, and can be a valuable tool for identifying process improvements that can result in fewer environmental burdens. A life cycle assessment will be conducted on a renewable hydrogen system, to complement the analysis of steam methane reforming, conducted in FY99. The assessment will include material and energy balances on all processes required for the process of interest, the hydrogen generation plant, to operate. Environmental stressors to be quantified include several air, water, and solid waste emissions, natural resource consumption, and energy use.

Task 5: Update of Hydrogen from Biomass - Determination of the Delivered Cost of Hydrogen

Previous analyses of the production of hydrogen from biomass will be updated to include recent experimental advances and changes in direction. The systems to be examined are gasification in the Battelle/FERCO gasifier followed by steam reforming, gasification in the IGT gasifier followed by steam reforming, and pyrolysis followed by coproduct separation and steam reforming. All analyses will include Monte Carlo sensitivity analysis.

Task 6: Analysis of the Production of Hydrogen from Air Products- SER and ITM Reactors

An independent appraisal of the technical and economic viability of reactors being designed by Air Products under DOE funding will be made. The technologies to be studied are the SER and ITM reactors, and the extent to which the analyses will project total costs will be based on the amount of data obtained from Air Products. Co-production of hydrogen and electricity, based on the work performed in FY99 by

Sandy Thomas, will be examined as an option for reducing the total cost of the product hydrogen. This study will also include an assessment of the technical and economic feasibility of hydrogen production via thermocatalytic cracking, as funded by the Hydrogen Program.

Task 7: Evaluation of Options for Photobiological Hydrogen Production

A full range of analyses will be completed for the various options to produce hydrogen photobiologically, including direct and indirect algal water splitting. Some analyses will be based on previous work, and will include advances made in the laboratory over the last few years. New projects funded by the Hydrogen Program in this area will be studied in as much detail as current research results will allow. Those projects that have generated enough information to complete a detailed analysis will be compared. All analyses will include detailed Monte Carlo sensitivity analyses.

Task 8: Comparison of On-board Hydrogen Storage

A literature review on currently-available hydrogen storage technologies will be conducted to compare system size, weight, and range to what can be achieved with gasoline. Systems to be examined include compressed gas, conformable tanks, metal hydrides, cryo-gas, and possibly carbon systems such as carbon nanotubes. The amount of hydrogen to be stored is 3.6 kg, which is sufficient for 360-380 miles in a fuel cell vehicle.

Distributed Hydrogen Fueling Systems Analysis - Directed Technologies, Inc. (DTI)

During FY '99 DTI began a new three-year contract to analyze and compare in detail the three major fuel options for fuel cell vehicles: hydrogen, gasoline and methanol. While DTI and others have analyzed some of the costs associated with providing fuel for fuel cell vehicles, additional analysis is required both to estimate the likely relative costs of these three fuels and also to design and engineer systems to reduce the costs of delivered hydrogen for fuel cell vehicles. In the second and third years, this project will concentrate on designing and developing small-scale, low-cost stationary hydrogen fueling systems.

Task 1: The Gasoline Option

Directed Technologies will estimate the annual investment costs made by the oil industry to maintain the existing gasoline infrastructure, including the prorated share of oil exploration and production. Directed Technologies will estimate the cost per gallon for providing essentially sulfur-free gasoline (less than one ppm), compared to the cost of removing the sulfur onboard each vehicle as part of the fuel processor and compare the cost per mile for a direct hydrogen FCV compared to a FCV with an onboard gasoline fuel processor operating on sulfur-free gasoline.

Task 2: The Methanol Option

Directed Technologies will estimate the cost of installing a methanol distribution system, and estimate the cost of methanol based on existing methanol production capacity and estimate the long-term methanol investments required to build new production capacity once existing surplus capacity is consumed by new demand.

Distributed Hydrogen Fueling Systems Analysis
Directed Technologies, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Gasoline Option						
Complete analysis				◆		
Methanol Option						
Complete data collection & analysis			◆			
Hydrogen Option						
Complete analysis					◆	

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Task 3: The Hydrogen Option

Directed Technologies will analyze the optimum fast-fill fueling option for compressed hydrogen, exploring in detail the mix of cascade and booster compressor filling suggested by Tom Halvorson of Praxair. The company will incorporate the optimum fueling system into the previous DTI economic model to estimate the cost of delivered hydrogen. Directed technologies will evaluate the electrical grid mix required such that electrolytic hydrogen consumed in a FCV would produce less greenhouse gases than a conventional gasoline ICEV, and estimate which US utilities will likely meet this criterion in the next few decades. Directed Technologies will also determine what utility conditions are necessary such that cogeneration of electricity at a local hydrogen fueling station would improve project economics over providing hydrogen fuel alone.

Hydrogen Energy System Studies – Princeton University

Researchers at Princeton Center for Energy and Environmental Studies will carry out a series of detailed technical and economic assessments with the goal of understanding the prospects for hydrogen fueled PEM fuel cell cogeneration technology for residential applications. Princeton University will compare three types of PEM fuel cell cogeneration systems which could provide heat and power to residential users:

Princeton University will compare three types of PEM fuel cell cogeneration systems that could provide heat and power to residential users.

Case 1) A centralized "neighborhood" scale (200-1000 kW) natural gas reformer/PEM fuel cell system which distributes heat (via district heating) and electricity (via wire) to 40-200 residential users.

Case 2) A centralized "neighborhood" scale natural gas reformer, which produces hydrogen or a hydrogen rich gas for distribution to users. Each house has a small hydrogen fueled (5 kWe) PEM fuel cell providing electricity and heat.

Case 3) Individual natural gas reformers coupled to 5 kW PEM fuel cells at each house.

For each case energy storage (in the form of hydrogen storage, hot water storage or electric batteries) could be used to meet time varying energy demands. Connections to the electric utility system could be made at the household or neighborhood level, allowing dispatch of power.

In the proposed work, engineering and economic models of PEM fuel cell based cogeneration systems will be developed. The potential advantages and disadvantages of each configuration will be investigated in terms of overall energy efficiency, performance, economics (capital cost, delivered cost of electricity and heat), and greenhouse gas emissions. PEMFC cogeneration systems will be compared to other alternatives for production of residential heat and power.

Hydrogen Energy Systems Studies
Princeton University

		2000				**2001**
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Design Trade-Offs						
Investigate design trade-offs				◆		
Costs and Trade-Offs Involved in Distributing Energy						
Discuss trade-offs for distributing various forms of energy				◆		
Cost of Electricity and Heat from PEM Fuel Cells						
Estimate cost of electricity and heat from fuel cells				◆		
Analyze the Role of Distributed & Emissions Benefits						
Discuss the benefits of fuel cells					◆	

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Task 1: Develop engineering models of various types of PEM fuel cell cogeneration systems capable of supplying residential heat and power

Existing data base on performance and cost of system components such as PEMFC stacks, small natural gas reformers and power electronics will be updated and extended to include small systems (3-5 kW). Where appropriate engineering models of components such as fuel cell stacks and reformers will be developed, drawing on related work Princeton University has done as part of its PEMFC vehicle modeling research. Heat-integrated PEMFC cogeneration system models will be developed using ASPEN software to model steady state performance.

Task 2: Component Sizing

Princeton University will develop component sizing algorithms for various types of PEMFC cogeneration systems, based on the demand profile, energy prices and component performance.

Task 3: Design Trade-offs

Princeton University will investigate design trade-offs that answer the following questions. What type of reformer technology is preferred? How do scale economies in reformer technologies, energy storage and power conditioning equipment effect the economics of combined heat and power generation? What are the effects of fuel cell operating pressure and temperature on the system design? What are the heat integration opportunities on each system's performance and cost?

Task 4: Discuss the Costs and Trade-offs Involved in Distributing Different Forms of Energy to Houses

Princeton University will assess the costs and trade-offs of three cases: case 1: electricity and hot water, case 2: hydrogen rich gas, case 3: natural gas.

Task 5: Cost of Electricity and Heat from PEM Fuel Cells

Princeton University will estimate the cost of electricity and heat from PEM fuel cells, as compared to alternatives.

Task 6: Analyze and Discuss the Role of Distributed Benefits and Emissions Benefits in the Economic Competitiveness of Fuel Cells

Princeton University will estimate the required component cost and performance goals for small scale PEMFC cogeneration systems to compete economically with alternatives, when distributed and emissions benefits are included. (This task will be performed in coordination with researchers at Distributed Utilities Associates).

Strategic Response to Scenario Planning - National Renewable Energy Laboratory

This effort stems from HTAP's recommendation in its Report to Congress that the "Hydrogen Program host vision setting/scenario development exercises, including workshops" to "develop compelling visions and scenarios of a hydrogen energy future. . . [that will] advance the concept of hydrogen energy to senior DOE management, the Congress, and the public" (Sec. 3.1). The scenarios will help to link HTAP's overarching vision and the Program's RD&D project portfolio by providing a "rationale" for the Program.

Scenarios are tools to provide a context to explore a chosen topic. In this effort, the topic is the DOE Hydrogen Program's RD&D portfolio. The purpose is to apply a scenario planning process to develop a long-term rationale for hydrogen RD&D sponsored by the DOE Hydrogen Program. The scenarios will be used by HTAP to influence government policymakers and Congress, and to engage and excite the public about the future of hydrogen. For instance, the stories will be used in preparing suggested topics for the reauthorization of the legislation and in the explanation of the need for a complex diversified program throughout government.

The report by the World Business Council for Sustainable Development (WBCSD) identifies three phases in scenario planning: Global Scenarios; Focused Scenarios; and Strategy Development. Given limitations of time and funding, NREL proposes that an abridged Phase 1 be conducted by gleaning what it needs from available scenarios, such as those developed by the WBCSD, the Intergovernmental Panel on Climate Change (IPCC), and the World Energy Council (WEC) under multi-year, multi-million dollar projects. NREL further proposes that the HTAP Scenario Planning Committee's effort should concentrate on Phase 2, Focused Scenarios. In the WBCSD process, the focused scenarios are specific to a corporation and set the context for business strategy. For HTAP, the focused scenarios will be energy and hydrogen-specific and will set the context for strategic planning by the Hydrogen Program.

Task 1: Scenario Development

Using NREL staff, HTAP's focused scenarios will be derived from the global scenarios prepared by the WBCSD, IPCC, WEC, and others by drawing out implications for energy in general and hydrogen in particular from these global scenarios. To abridge Phase 1, NREL will develop a set of scenario families and storylines, most likely three, from the WBCSD, IPCC, WEC, and other scenarios, including those drafted by Chris Flavin. This set will include bedrock assumptions, branching points, and dimensions of change derived from the source scenarios.

Strategic Response to Scenario Planning
National Renewable Energy Laboratory

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Focused Scenario Workshop						
Conduct workshop		◆				
Finalize HTAP scenarios					◆	
Strategic Response Workshop						
Conduct Strategic Response Workshop					◆	

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Task 2: Focused Scenario Workshop

At a workshop held in conjunction with the semiannual HTAP meeting, NREL will draw out enough of the details of the storylines to make them compelling and interesting to its client and to other key constituencies. NREL will also discuss in depth the branching points and the dimensions of change that may interact and lead to different futures and will “name” the scenarios. NREL will synthesize the discussion and outputs of the workshop into draft HTAP scenarios.

Following a review by HTAP, DOE, and other key organizations, the scenarios will be revised and presented to the public (by HTAP) in April 2000 in conjunction with an appropriate Earth Day event. After the HTAP scenarios are presented, they will be validated in meetings with key constituencies, such as senior DOE management, Congressional staffers, industry, and public interest groups. The validation process should be useful to HTAP in reauthorizing the Hydrogen Futures Act and in the FY 2001 budget process. Once validated, the scenarios will be formally adopted by the HTAP and transmitted to the DOE Hydrogen Program.

Task 3: Strategic Response Workshop

After adoption and transmittal of the scenarios, HTAP, DOE, NREL, and other national laboratories will convene a workshop to develop strategic responses to each of the HTAP scenarios. Given the futures identified in the scenarios, the participants will develop strategies for the DOE to achieve the overarching HTAP vision of hydrogen being one of two principal energy carriers in the 21st Century. The strategic responses will focus on opportunities for hydrogen, key barriers, strengths and weakness of the Program to seize the opportunities and overcome the barriers, and to identify RD&D needs and priorities.

Table 3.7 Technology Transfer Projects		
Goal: Develop informed constituencies in the industrial and public sectors as part of a strategy to accelerate the commercialization of renewable hydrogen technologies		
Category	**Project**	**Research**
Technology Transfer Activities	International Energy Agency and Other International Collaborations	National Renewable Energy Laboratory
	IEA Support	Energetics, Inc.
	HTAP Coordination	National Renewable Energy Laboratory
	Outreach Activities	National Hydrogen Association
	Education Outreach	MRS Enterprises
	Outreach Activities	Sentech, Incorporated
	Raising Awareness of H_2 in The Technical Community	Energetics, Inc.
	The H2000 Project	H2000

TECHNOLOGY TRANSFER ACTIVITIES

International Energy Agency and Other International Collaborations - National Renewable Energy Laboratory

The objective of this project is to foster international collaborations and technology transfer for the advancement of hydrogen production, storage and utilization technologies. Included is support for activities conducted within the framework of the International Energy Agency (IEA). NREL provides the Secretariat function, as well as the Task Leader for the Integrated System activities and experts for the Photoelectrochemical Hydrogen Production, Carbon for Hydrogen Storage and Integrated Systems tasks, all for the IEA Hydrogen Agreement and provides an expert on biomass pyrolysis and pyrolysis oils for the IEA Bioenergy Agreement. This project also provides support for two international collaboration: (1) with the University Rovira i Virgili, Spain, to develop steam reforming of bio-oil and (2) with the University of Montpellier II, France, to further develop NREL's expertise in carbon nanotube production technology for the purposes of hydrogen storage. Finally, the project provides the U.S. liaison to the International Gas Union.

Task 1: Secretariat support

NREL serves as the administrative arm of the Executive Committee, and is responsible for the day-to-day operations of the Implementing Agreement. This includes organizing and reporting on the Executive Committee meetings, producing the Annual Report, managing the Common Fund, and monitoring the activities of all Annex activities.

International Energy Agency and Other International Collaborations
National Renewable Energy Laboratory (NREL)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Secretariat Support						
Arrange fall 1999 Executive Committee Meeting		◆				
Arrange spring 2000 Executive Committee Meeting				◆		
Participation in IEA Hydrogen Annex 13 Activities						
Complete report 1 on revised and new component models		◆				
Complete report 1 on cost models		◆				
Conduct cost analysis for LCA of conventional system				◆		
Report on first optimized integrated advanced system				◆		
Complete economics and infrastructure chapter for IGU				◆		

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Task 2: Integrated Systems Annex 13 operations

The objective of Annex 13, Design and Optimization of Integrated Systems, is to develop a tool to assist in the design and evaluation of potential hydrogen demonstration projects and in the optimization of existing hydrogen demonstration projects. Emphasis will be placed on integrated systems covering all components, from input energy to end use. The activities will be focused on near- and mid-term applications, with consideration of the transition to sustainable hydrogen energy systems. Component models developed under a previous task will be updated and refined to include cost information. Finally, life cycle assessments will be performed on comparative hydrogen systems.

NREL serves as the Operating Agent (OA) for Annex 13. In this capacity, overall organization and technical and administrative management of the activity are required. In addition, the OA is required to report on a regular basis to the Executive Committee, and to provide detailed reports as stipulated in the Annex 13 work plan.

Task 3: Participation in IEA Hydrogen Agreement Annex 13 Activities

Existing and proposed hydrogen energy system demonstrations typically deploy technologies at different levels of development. A combination of data collection, demonstration case studies, component simulation, integrated systems modeling and life cycle assessment will result in the development of design guidelines for future demonstrations.

NREL expertise in process simulation and analysis are critical to the success of this activity. Participation is required in Subtask A (Model Development) and Subtask B (Systems Analysis) of Annex 13.

IEA Support – Energetics, Inc.

The U.S., through the DOE Hydrogen Program supports several annexes of the International Energy Agency (IEA) Hydrogen Implementing Agreement. This includes Annex 13 on Design and Optimization on Integrated Systems which was started in December, 1998, building on the successes of the previous Integrated Systems annex – Annex 11. One function of participants in Annex 13 is the role of “expert” to participate in the development and optimization of a tool that will assist in the design and evaluation of potential hydrogen demonstration projects and optimize existing projects.

Since the inception of Annex 13, Energetics has been designated the Activity Leader for Activity A1: Component Model Development and Improvement. This Activity involves the additional of several new models to the component library, and the revision of Annex 11 models, as necessary, based on new or improved data. In addition, the Activity A1 Leader must work closely with the activity B1 Leader in determining the level of integration needed within the component models and its effect on the system integration.

Task 1: Identification of Component Process and Coordination

The task for the IEA Annex 13 Project in FY 2000 involves the identification of new or revised component process and the coordination of its development as an ASPEN Plus® model for Activity A1, as well as working closely with the Activity B1 leader to provide input to systems optimization, and providing engineering input to the other Annex activities on life cycle analysis, and especially cost model development.

New/revised models that are of interest include those for: pressure swing adsorption (PSA), membranes, and the production processes that would now be decoupled from these purification processes (e.g., coal gasification, biomass gasification, biomass pyrolysis, etc.) In order to best address (and keep current with technology for) these new models, Energetics will work with those members of the US Hydrogen community engaged in thermal (fossil or biomass-based) hydrogen production and purification in order to develop more accurate input to be used to upgrade the component models.

Energetics, acting as Annex 13 Activity A1 Leader will identify and coordinate the construction of new component models. The contractor will also coordinate the revision of existing models as necessary to reflect the existence of new or improved data. The contractor will also work with the Activity Leaders of the other activities to provide engineering input to cost models, life cycle analyses, and systems integration as required. The contractor will participate in two Experts’ Meetings during FY 2000. The Spring 2000 Experts’ Meeting is tentatively scheduled for April in Amsterdam, The Netherlands. The site and date of the Fall 2000 Experts’ Meeting has been tentatively scheduled for Munich, Germany in September. This meeting will coincide with the Hyforum 2000 meeting.

IEA Support
Energetics, Inc.

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Identification of Component Process and Coordination						
Attend Annex 13 Spring Experts' Meeting				◆		
Attend Annex 13 Fall Experts' Meeting					◆	

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HTAP Coordination - National Renewable Energy Laboratory

The Hydrogen Technical Advisory Panel (HTAP) was authorized by the Matsunaga Act of 1992 and reauthorized by the Hydrogen Future Act of 1996. The Panel serves in an advisory capacity to the Secretary of Energy, providing insight into research and development requirements for the transition to a hydrogen economy.

Two HTAP meetings per year are held, with one generally held in conjunction with the National Hydrogen Association's Annual Meeting (in the Washington, DC area in the spring). The second meeting is held in different locations to increase the accessibility of the Panel to the general public. The panel also holds special international discussions at appropriate international meetings, such as the World Hydrogen Energy Conference and the HyForum conference.

In addition to these full-panel meetings, a number of committees have been formed to develop more detailed information on specific topics of interest to the Panel and DOE. The committees meet once per year, or as necessary.

Task 1: Logistic Support

NREL provides logistic support for the coordination of the meetings, and also provides technical and clerical assistance as necessary. This includes reimbursing HTAP members and certain invited guests for their travel expenses.

Task 2: HTAP Meeting Minutes

NREL provides a report of the complete minutes and a condensed report to the DOE Designated Federal Official, as required by advisory panel regulation.

HTAP Coordination
National Renewable Energy Laboratory (NREL)

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Logistic Support						
Arrange fall 99 HTAP meeting		◆				
Arrange spring 00 meeting			◆			
HTAP Meeting Minutes						
Write Fall 99 HTAP meeting minutes and report		◆				
Write spring 00 HTAP meeting minutes and report				◆		

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Outreach Activities – National Hydrogen Association

The NHA looks to foster the development of hydrogen technologies and their utilization in industrial and commercial applications and to promote the transition of hydrogen in the energy field. In order to facilitate hydrogen's acceptance in the public arena, the NHA will conduct outreach activities to educate and make the public aware of hydrogen's potential.

Task 1: NHA Information Exchange

The NHA will continue efforts to analyze current domestic and international hydrogen technology development and develop a timely information exchange method to provide current information on technology research and development. The NHA will disseminate this information to the hydrogen industry, utilities, project developers, and state and local officials through various mechanisms, such as publications, workshops, and the Internet.

Task 2: Hydrogen Joint Working Group of the Americas and Pacific Rim

The NHA will take the lead in coordinating with other countries in Canada and the Pacific Rim to form a Joint Working Group of Hydrogen Associations. This is not meant to replace the national hydrogen associations whose goals concern hydrogen economic interests of their respective countries. Instead it is aimed at multinational cooperation and the exchange of information which each member organization can use for their own benefit. It may also have a role in helping countries, that request it, develop a nation association that country's energy needs. The group will develop a basis charter and annual plan for the Hydrogen Joint Working Group. It will develop a program plan and budget for the Hydrogen Joint Working Group. It will also conduct an organizational meeting and conduct the first joint working group meeting. It will also prepare and present a paper on the Hydrogen Joint Working Group at Hyforum 2000.

Task 3: Annual U.S. Hydrogen Meetings

The NHA will conduct the *11th Annual U.S. Hydrogen Meeting* from February 29-March 2, 2000.

Outreach Activities – National Hydrogen Association

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
NHA Information Exchange						
Hold implementation plan meeting in Tahoe City, CA		◆				
Complete H2 brochure and power point slide library				◆		
Hydrogen Joint Working Group						
Conduct first organizational meeting			◆			
Develop joint working group program plan and budget			◆			
Approve charter			◆			
Conduct the first joint working group meeting				◆		
Prepare and present paper at Hyforum 2000					◆	
Annual U.S. Hydrogen Meetings						
Conduct the 11th Annual U.S. Hydrogen Meetin			◆			

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Education Outreach – MRS Enterprises

The Education Outreach Project is intended to teach students about the potential of hydrogen as a fuel and an energy carrier. Its activities build on the PI's efforts which began in FY '97. The Education Outreach Project complements related Hydrogen Program activities such as development of the CD ROM. An important theme of the 'FY 2000 Education Outreach Project will be a coordinated approach to promotion of its education products and activities. Contemplated FY2000 activities include: assembly and packaging of curriculum (print and film); formal curriculum field-testing; formulation of a distribution strategy using a mixed print and web-based solution; and enhancement of established education outreach events such as the *Dr. Bob Show* at the NHA Conference.

Task 1: Clean Corridor Curriculum (CCC)

Subtask 1.1: The High School *Clean Corridor Curriculum*
The curriculum, revised during an FY'99 summer workshop, will be reviewed and modified for technical accuracy. It will then become the subject of a national field-test. Aimed at first year high school chemistry students, the *CCC* now contains six modules: Fundamentals; Production; Storage; Distribution and Safety; Utilization; and Mission H_2 in addition to the final project, *Hydrogen Filling Station Project*. All modules were expanded. All modules were expanded. The curriculum is intended as a complement and enrichment to both traditional and innovative approaches to chemistry. Its modular structure — topical modules broken into lessons with over 50 student activities — lends itself to flexible integration with other instructional materials. In its entirety, the curriculum provides 90 hours of classroom instruction and covers 80-85% of national science standards for chemistry.

Subtask 1.2: The Middle School *Clean Corridor Curriculum*
The existing high school curriculum will be modified during an FY'99 summer workshop, then subject to technical review. This product is intended to be appropriate for middle school populations. Funding permitting, field-testing of this beta curriculum will take place and the curriculum will be revised to incorporate its field test feedback during a summer 2000 workshop.

Education Outreach
MRS Enterprises

Task Designation/ Milestone		2000				2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Clean Corridor Curriculum						
Revise high school Clean Corridor Curriculum		◆				
Make school hydrogen curriculum available			◆			
Report on field test and teacher training					◆	
Videos and Video Clips						
Write, produce and edit Beakman on H2 film				◆		
Science Shows						
Complete Secondary School Invitational with Dr. Bob Show					◆	

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Subtask 1.3: Curricula dissemination, a multi-part activity. The first dissemination activity entails field-testing and evaluation of the high school *Clean Corridor Curriculum.* Field-testing and evaluation is expected to occur in several geographic regions and school systems, including both public and private schools. Participating teachers will receive a stipend for completion of field-test activities. Funding permitting, a workshop will be held during the summer of 2000 to revise the product. In the event it occurs, it will include development of material on micro-gravity per instructions of the Annual Program review.

Subtask 1.4: Teacher Training. Selected teacher training will continue through teacher in-service days (as funding permits) and conference participation. Certain conferences such as the Maryland Association of Science Teachers Conference and the National Science Teachers Association Conference offer excellent forums for curriculum promotion and dissemination and possible teacher training. Participation in other conferences and training opportunities will be explored and pursued, funding permitting.

Subtask 1.5: Reproduction of the *Clean Corridor* Curriculum. Hard copies of the *Clean Corridor Curriculum* must be reproduced and distributed. Appropriate curriculum announcements will be developed to support distribution. Notice of curriculum availability and the field test will be posted on the NREL hydrogen web site together with selected content from the curriculum. A new M.R.S. Enterprises web site directed to education outreach will be constructed, funding permitting. An end-to-end distribution strategy for the curricula will be developed for both curricula and implemented for the high school Clean Corridor Curriculum, funding permitting.

Subtask 1.6: Develop and Disseminate a Reversible Fuel Cell Demonstration Unit
Funding permitting, M.R.S. will develop and disseminate a reversible fuel cell demonstration unit as part of the Deluxe Teachers Kit for the *Clean Corridor Curriculum*. Teachers and schools participating in the *Clean Corridor Curriculum* field test will receive priority consideration in distribution of these demonstration units.

Task 2: Videos and video clips

MRS Enterprise will write, produce and edit Paul Zaloom in *Beakman's World: Beakman on Hydrogen*. Building on the FY'99 video products and *Beakman's World: Beakman on Hydrogen*, MRS Enterprises will explore other film and TV production opportunities involving both the *Dr. Bob Show* and the *Clean Corridor Curriculum.* Pursue such opportunities as funding permits.

Task 3: Science Shows

The Dr. Bob Show*,* an established feature of the Education Outreach Task, offers continuing opportunities for education outreach as both a live (at the 11th Annual National Hydrogen Association Conference) and a filmed production.

Research and pursue other opportunities for live science shows as funding permits.

Task 4: Challenge Grants

A Challenge Project that offers monetary grants will support secondary school hydrogen demonstrations. The selection process will give priority to teachers and schools participating in the field test.

Task 5: Hydrogen Education Outreach Coordination

Funding permitting, a comprehensive education outreach plan will be developed to assure coordination of all activities and provide a vehicle for enhancement of education outreach.

Outreach Activities – Sentech, Incorporated

The objectives of Sentech's activities is to develop the tools necessary to convey to multiple audiences (including industry, policy decision makers, educators, and the public) the objectives and content of DOE's Hydrogen Program.

Sentech has been tasked to facilitate the Program's activities in education and public awareness to increase understanding of the merits of hydrogen by developing innovative materials that describe the characteristics of hydrogen energy systems and their role in a sustainable energy economy. Sentech's outreach activities are expected to lead to increased understanding between DOE and its audiences so that areas of common interest can be developed into well-defined projects for hydrogen technology development and deployment. The efforts to be conducted during the first quarter of FY 2000 are focused on the integration of hydrogen energy systems into the Nation's infrastructure.

Task 1: Industry Outreach

A key to successful hydrogen energy systems is to overcome barriers, such as a lack of hydrogen availability, refueling stations, and safety provisions. There are a number of public and private sector efforts currently underway to address these barriers. Sentech is assisting NREL in conducting an interactive workshop in late October 1999 with key industry decision-makers defining the steps required to achieve a hydrogen infrastructure. Discussions will include the creation of a structured timeline for the technologies necessary throughout the development of the infrastructure system. A draft blueprint and timeline will be produced in December of 1999, reviewed, then produced in final form by March 2000, thereby providing information to both industry and government to further the progress of hydrogen technologies.

Outreach Tasks
Sentech, Incorporated

		2000				2001
Task Designation/ Milestone	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Industry Outreach						
Conduct workshop		◆				
Deliver final draft blueprint		◆				
Deliver industry meeting analysis paper			◆			
Deliver industry meeting analysis paper		◆				
Education						
Deliver final teacher's guide		◆				
Deliver experiment sheets		◆				
Deliver draft marketing and distribution plan		◆				
Conclude field testing of CD-Rom				◆		
Unveil mission H2 CD-Rom on earth day 2000				◆		
Awareness						
Deliver project fact sheets		◆				
Deliver final draft of outreach opportunity document		◆				

FY 2000 Begins October 1, 1999

Sentech has also been tasked to revisit the industry outreach meetings that were conducted in 1995/96. The primary purpose of which is to update and further educate those industry groups (or companies) less involved in the hydrogen arena on current Hydrogen Program activities. Sentech will conduct a series of phone interviews and select 4-6 companies within the original group with which to organize individual industry meetings. The discussions will be documented in individual trip reports, and will include an analysis of change in industry direction since the previous meetings to be delivered in December of 1999.

Task 2: Education

With the completion of the *Mission* H_2 CD-ROM in FY '99, Sentech is developing a complete package, that will include a teacher's guide and several experiment sheets, to make available for teachers and students to learn about hydrogen energy. The development and testing of this supplemental package will occur during the first 2 quarters of FY 2000, and will be unveiled in the Spring of 2000. Sentech will also look into a variety of distribution channels resulting in a targeted marketing and distribution plan. All documents will be delivered in December of 1999.

Task 3: Public Awareness

The FY '99 awareness task was successful in providing valuable information on the many positive aspects of hydrogen as an energy carrier to the general public and industry groups. The results of the FY '99 outreach activities will continue to impact the development of supplemental documents and interactive exhibit components in the first quarter of FY 2000 to further focus the message to the general public, industry, educational institutions, state and local agencies, and other specific audiences. The following are deliverables for the first quarter of FY 2000:

<u>Subtask 3.1: Prepare three one-page project fact sheets</u>
Sentech will prepare the fact sheets (including the three produced in FY '99) as the foundation for a new outreach document that will effectively communicate to industry groups and others the successful opportunities that hydrogen technologies offer.

<u>Subtask 3.2: Develop additional components for use in the exhibit display to better focus the message for a variety of audiences.</u>
The supplemental components will provide a quick cost-effective means of changing the appearance of the exhibit display and the subsequent message that is presented.

<u>Subtask 3.3: Promote awareness and benefits of hydrogen as an energy carrier</u>
Sentech will promote the future benefits that hydrogen technologies will provide to stakeholders by utilizing the exhibit display at additional m

Raising Awareness of H_2 in the Technical Community – Energetics, Inc.

The need for clean, inexpensive energy in the 21st century has led both the public and private sectors to vigorously pursue the research, development, and validation of hydrogen technologies. Yet many entities are unaware of the current status of the technologies that will enable hydrogen as an energy carrier, and what work still needs to be done. Many of these entities, some U.S. universities for example, have the potential to contribute greatly to hydrogen technologies development, if provided with the proper information. The proposed work will provide the existing hydrogen community, and those that plan to become involved, with the status of several critical hydrogen technologies currently being developed at the R&D, validation, and systems levels. At the same time, it will provide the academic community with a better understanding of the gaps in hydrogen R&D, which will help focus university R&D in the directions needed to make hydrogen a prominent energy carrier.

In order to provide timely and accurate information on the status of hydrogen technologies to the public, especially those entities that may be considering the undertaking of hydrogen activities, it is necessary to review these technologies on a scientific and engineering basis. The contractor will perform a series of independent technical assessments aimed at defining the key parameters needed to further the role of hydrogen in the future energy mix, and provide reports on these issues to the public.

Task 1: Technical Assessments of Hydrogen R&D Technologies

Energetics will assess critical technologies on specific hydrogen production, storage, and utilization R&D projects. Energetics, having identified several key hydrogen technologies that are currently being developed by the DOE Hydrogen Program, will review existing literature and prepare a list of technical questions that will serve as the basis of extensive discussions with the Principle Investigators, and will undertake site visits. The information base thus generated will be the basis of a technical evaluation of the concept, and will be used to generate reports to the public that will discuss the technologies on the basis of status and need. This information will also be made available to the review panels for the Hydrogen Program Annual Peer Review. Currently, three evaluations are planned. The identification of the three projects will in part be based on comments made by the FY1999 Peer Review Panel.

The H2000 Project – H2000

INPUT NOT RECEIVED

Raising Awareness of H_2 in the Technical Community
Energetics, Inc.

Task Designation/ Milestone		2000				2001
	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1
Technical Assessments of Hydrogen R&D Technologies						
Identify projects		◆				
Complete 1st evaluation			◆			
Complete 2nd evaluation			◆			
Complete 3rd evaluation				◆		

FY 2000 Begins October 1, 2000

4.0 STATUS AND PLANS

4.1 National Recognition

As the Hydrogen Program has grown in size over the past several years, so has it grown in stature as seen by the year-to-year increase in the number of patents, patent applications, awards, and other forms of recognition of achievement. These merits are itemized in this section.

FY 1994

P. Weaver, and P. -C. Maness, "Photoconversion of Gasified Organic Materials into Biologically Degradable Plastics," U.S. Patent 5, 250,427, issued October 5, 1993.

Dr. P.F. Weaver and his NREL research group also have a patent pending entitled, "Photoconversion of Gasified Organic Materials into Single-Cell Protein."

C. Linkous, "Apparatus and Method for the Electrolysis of Water Employing a Sulfonated Solid Polymer Electrolyte," U.S. Patent 5,271,813, issued December 21, 1993.

Dr. Linkous also received the 1994 Distinguished Researcher Award from the University of Central Florida Centers and Institutes.

FY 1995

Midwest Research Institute's *President's Award* was presented to Dr. John Turner (NREL) for exceptional performance, 1995.

Dr. Eli Greenbaum of ORNL received the 1995 DOE Biological and Chemical Technologies Research Program Technical Achievement Award.

Patent applications or disclosures were filed for the following:

University of Hawaii - patent application:

- Antal: Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

Oak Ridge National Laboratory - patent application:

- J. Woodward, S. Mattingly, and M. Danson "An Enzymatic Process for the Generation of Molecular Hydrogen from Glucose";

National Renewable Energy Laboratory - invention disclosure:

- D. Benson, Disclosure to NREL patent office on new design for chemochromic hydrogen detector;

Sandia National Laboratories - 3 patent disclosures:

- G. Thomas, "Metal alloy for hydrogen storage,"
- G. Thomas, "Process for manufacturing hydride beds," and
- G. Thomas, "Synthesis of magnesium alloys with controlled phase."

Energy Conversion Devices, Incorporated - patent application:

- K. Sapru et al. "Magnesium Mechanical Alloys for the Thermal Hydrogen Storage," Patent application serial number 08/363,205, filed 22 Dec. 1994.

FY 1996

Dr. M.J. Heben NREL) was invited to perform research in solar production of carbon nanotubes in France at The Universite Montpellier II by the French Ministry of Foreign Affairs.

M. L. Ghirardi and M. Seibert (NREL) filed a Record of Invention Report (NREL No. 96-46) entitled "A Technique Based on H_2-Production Pressure to Select for Algal Mutants that Produce Hydrogen Under Aerobic Conditions", July 1996.

Dr. P.F. Weaver (NREL) filed a U.S. patent application entitled "Photoconversion of Thermally Gasified Biomass into Single-cell Protein."

Dr. Jonathan Woodward (ORNL) applied for a patent entitled "Enzymatic Method for Hydrogen Production from Glucose. U.S. patent application, esid-1833-x.

Dr. David Benson (NREL) filed a patent application “Fiber Optic Sensing Device” (May 1996)

Dr. Benson was also recognized by the Hydrogen Technical Advisory Panel for "Ingenuity and Research Excellence in development of the fiber optic hydrogen sensor" (April 1996).

A U.S. Patent was awarded to Drs. C. Jensen and W.C. Kaska, University of Hawaii, entitled "Process for Alkane Dehydrogenation with Organometallic Catalyst," U.S. Patent 5,687,717.

Members of the Air Products and Chemicals, Inc. SER group have two patents pending:

Nataraj, S.N., Carvill, B.T., Hufton, J.R., Mayorga, S.M., Gaffney, T.R., and Brzozowski, J.R., "Process for Operating Equilibrium Controlled Reactions," U.S. Patent Pending (1996).

Mayorga, S. G., Golden, T. C., Gaffney, T. R, Brzozowski, J. R., and Taylor, F. W., “ Carbon Dioxide Pressure Swing Adsorption Process Using Modified Alumina Adsorbents,” U. S. Patent Pending (1996).

C. Zawodzinski and M.S. Wilson, LANL, submitted a Formal Disclosure to the LANL Patent Office entitled "Stainless Steel Wire Mesh Flow Fields for Polymer Electrolyte Fuel Cells", November 1995.

The following recognition was afforded SERC's Palm Desert Project:

- The British Broadcasting Corporation's crew visited SERC and produced a clip that appeared during May 1996 on the BBC's show, *Tomorrow's World* .

- Newspaper and magazine articles: SERC's project was mentioned in numerous local, regional, national, and international newspapers. In addition, the December 1995 *Scientific American* ran an article about the Palm Desert Project.

- Demonstrations: Demonstrations of SERC's fuel cell powered PUV were conducted for the President of the AAA (American Automobile Association), commissioners of the CEC (California Energy

Commission), the Chairman of the Board of CARB (the California Air Resources Board), at the Sacramento Municipal Utility District's Clean Power Day, at the Los Angeles Fleet Auto Show/Eco Expo, and at the City of Palm Desert's Clean Power Day.

Dr. Clovis Linkous (FSEC) was awarded U.S. patent #5,518,992, for "Photocatalytic Surfacing Agents for Inhibiting Algae Growth," May 21, 1996.

SNL has filed a patent disclosure entitled:

- "Continuous Microcellular Interstitial Media as an Immobilization Matrix,"

Energy Conversion Devices, Incorporated have filed the following patent applications:

- K. Sapru et al. "Robust Metal Hydride Hydrogen Storage System," Patent application serial number 08/569,487, filed 08 Dec. 1995.

- K. Sapru et al. "Robust Metal Hydride Hydrogen Storage System with Metal Support Structure," Patent application serial number 08/623,497, filed 03 Mar. 1996.

Dr. J. Bellan was awarded the Exceptional Service Award for Technology and Applications Programs from the Jet Propulsion Laboratory. The inscription reads: "In recognition of exceptional contribution in multiphase and reactive flows and combustion phenomena that have wide range of application in propulsion and aircraft engine design".

FY1997

Drs. M. L. Ghirardi and M. Seibert (NREL) filed a Patent Application on the invention entitled "A Technique Based on H_2-Production Pressure to Select for Algal Mutants that Produce Hydrogen Under Aerobic Conditions", April 1997.

Dr. Michael Seibert has received an NIS-IPP grant to work with a Russian group on a project that will support the Hydrogen Program's biohydrogen efforts.

Dr. Seibert also received an invitation from a Spanish Laboratory to give a seminar with travel expenses paid by the Spanish government.

Dr. Seibert's group also received a request from a Swiss National to join the group as a postdoctoral fellow at the expense of the Swiss government.

Dr. John Turner (NREL) and Dr. Rick Rocheleau (U Hawaii) were co-recipients of the HTAP second annual Hydrogen Program Research Success Story Award for work on "Photoelectrochemical Systems for the Production of Hydrogen".

Dr. David Benson (NREL), who has patent application for his Hydrogen sensor in the FY 1996 listings, has also applied for an international patent. The patent application was issued in October, 1997 as International Publication Number WO 97/37258. This is the first step in the process of obtaining international patents. Designated countries include Belgium, Switzerland, Denmark, Finland, Great Britain, Italy, Netherlands, Austria, Ireland, Spain, Australia, France, Luxenbourg, Monaco, Portugal, Germany, Greece, Australia, Japan, and Canada.

Dr. George Thomas (SNL) has filed a patent disclosure concerning an immobilization method for a hydride bed.

Dr. Craig Jensen and his associates at the University of Hawaii have filed the following two patent applications on polyhydride storage complexes:

"Process for Alkane Dehydrogenation with Organometallic Catalyst." W. Kaska and C. Jensen; U.S. Patent 8,687,717 filed July 1996.

"Low Temperature Catalytic System fo Chemical Storage of Hydrogen" Craig M. Jensen; U.S. Patent 8,807,123 filed February 1997.

Dr. Clovis Linkous of FSEC was awarded the Orlando Section of the American Chemical Society's "Outstanding Chemist Award in December 1996

The SERC/Palm Desert Project has gained additional exposure to that which was reported in FY 1996:

Articles about the project have appeared in:

Popular Science (September 1996, October 1996)

Motorland Magazine -a publication of the American Automobile Association (Nov/Dec 1996)

Wired Magazine (October 1997)

A video about the project has appeared on *Understanding Cars,* The Learning Channel, May, 1997

Oak Ridge National Laboratory Awards Night, "Technical Achievement Award, Invention" May 1997 to B. S. Hoffheins, R. J. Lauf, and P. H. Fleming.

F. Mitlitsky, B. Myers, and F. Magnotta, LLNL have filed an invention disclosure, "Lightweight bladder lined pressure vessels," *Disclosure and Record of Invention*, DOE Case No. IL-9722 (1995).

The Savannah River Bus Project was awarded the Federal Laboratory Consortium "1996 Southeast Regional Partnership Award"

Personnel involved with the Savannah River Bus Project were awarded the "Keys to City of Augusta", by Mayor Larry Sconyers and Senator Sam Nunn (D-GA).

C. Zawodzinski and M.S. Wilson, of the LANL PEM Fuel Cell Team have submitted a patent application to the US Patent Office entitled "Stainless Steel Wire Mesh Flow Fields for Polymer Electrolyte Fuel Cells."

Drs. J. Bellan and R. S. Miller were awarded NASA Certificates of Recognition (recognition for best and most important papers within NASA) were awarded for the following publications:

- "Analysis of Reaction Products and Conversion Time in the Pyrolysis of Cellulose and Wood Particles"
- "A Generalized Biomass Pyrolysis Model Based on Superimposed Cellulose, Hemicellulose and Lignin Kinetics"
- "Tar Yield and Collection from the Pyrolysis of Large Biomass Particles"

(See Section 4.4 for publication details)

An additional paper, "Numerical Simulation of Vortex Pyrolysis Reactors for Condensable Tar Production from Biomass," is currently also being considered for a NASA Certificate of Recognition.

Dr. Jonathan Woodward (ORNL) was awarded the Columbus Award for his glucose to hydrogen work

FY 1998

Oak Ridge National Laboratory

The ORNL Team won a Lockheed Martin Energy Research, Corp. invention award at the 1997 Awards Night.

National Renewable Energy Laboratory

Weaver, P.F., "Photoconversion of Thermally Gasified Biomass into Single-cell Protein." U.S. Patent application filed and appeal defended.

A Notice of Allowance was received from the US Patent Office regarding M. L. Ghirardi and M. Seibert's Patent "Process for Selecting Oxygen Tolerant Algal Mutants that Produce H_2 under Aerobic Conditions" in July, 1998.

A Patent Application on an invention entitled "A Chemochromic Sensor for Rapid Biohydrogen Phenotypic Screening" by M. Seibert, T. Flynn and D. Benson was filed in May, 1998.

Fiber Optic Device for Sensing the Presence of a Gas, David K. Benson, Clemens S. Bechinger and C. Edwin Tracy, US Patent No. 5,708,735, January 13, 1998.

NREL filed a provisional patent application on a closely related hydrogen sensor that is being successfully used by NREL bio-hydrogen researchers to facilitate the selection of hydrogen-producing mutant algae.

Los Alamos National Laboratory

M.S. Wilson and C. Zawodzinski, "Stainless Steel Wire Mesh Flow-Fields for Polymer Electrolyte Fuel Cells," Patent issued by the US Patent Office (No 5798187, Aug 25, 1998).

Lawrence Livermore National Laboratory

F. Mitlitsky, B. Myers, and F. Magnotta, “Lightweight bladder lined pressure vessels,” *Disclosure and Record of Invention*, DOE Case No. IL-9722, U.S. Patent No. 5,798,156, August 25 (1998).

F. Mitlitsky, J.B. Truher, J.L. Kaschmitter, and N.J. Colella, “Fabrication of polycrystalline thin films by pulsed laser processing,” *Disclosure and Record of Invention*, DOE Case No. IL-9123, U.S. Patent No. 5,714,404, February 3 (1998).

filed patent on electrolyzer concept

University of Hawaii

M.J. Antal: Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

M.J. Antal, X. Xu: Catalytic Supercritical Gasification of Biomass Starch Pastes, U.S. Provisional Patent Application.

Patent 5,780,701 Process for Alkane and Alkyl Group Dehydrogenation with Organometallic Catalyst; Craig M. Jensen, and William C. Kaska. Issued 7/98.

Sandia National Laboratories

- Patent Disclosures and Status
  Bed Immobilization Method – nearing completion
  Mg alloy – re-submitted

University of Miami

The Hydrogen Technical Advisory Panel (HTAP) awarded the Safety Analysis work at the University of Miami their Research Excellence Award on March 3, 1998 at the 9th Annual US Hydrogen Meeting

Savannah River Technology Center

Invention disclosure filed for membrane separation system.

ECD

Two patent applications filed: (a) "Metal Hydride Storage Container with Valved Ports", filed 1/20/98, and (b) "Self-Heating Metal Hydride Hydrogen Storage System," filed 2/13/98.

FY 1999

Massachusetts Institute of Technology

A patent application based on the novel plasma reformer was filed with the US patent office.

Paper presented at the Fall Meeting of the American Chemical Society was nominated for the Glen Award.

Lawrence Livermore National Laboratory

Lightweight Bladder Lined Pressure Vessels F. Mitlitsky, B. Myers, and F. Magnotta, *Disclosure and Record of Invention*, U.S. Patent No. 5,798,156, August 25 (1998).

Fabrication of Polycrystalline Thin Films by Pulsed Laser Processing, F. Mitlitsky, J.B. Truher, J.L. Kaschmitter, and N.J. Colella, *Disclosure and Record of Invention*, U.S. Patent No. 5,714,404, February 3 (1998).

National Renewable Energy Laboratory

MRI elected title in an invention entitled "An Approach for Photo-Producing Large Amounts of Hydrogen Using Hydrogenase-containing Oxygenic Photosynthetic Organisms" by A. Melis, L. Zhang, J.R. Benemann, M. Forestier, M. Ghirardi and M. Seibert, April 1999.

A patent entitled "A Chemochromic Sensor for Rapid Biohydrogen Phenotypic Screening" by M. Seibert, D.K. Benson and T.M. Flynn was filed, May 1999.

Weaver, P.F. "Photoconversion of Thermally Gasified Biomass into Single-cell Protein." U.S. patent application filed and appeal defended.

Oak Ridge National Laboratory

Dr. James Weifu Lee received two significant awards in FY 1999: (1) a DOE Early Career Award for Scientists and Engineers and (2) a Presidential Early Career Award for Scientists and Engineers. Dr. Lee was honored in ceremonies at DOE headquarters and the Old Executive Office Building. The awards were presented by Secretary of Energy Bill Richardson and Presidential Science Advisor Neal Lane.

A patent application by Lauf, R.J. "Resistive Hydrogen Sensing Element," was filed May 10, 1999.

Sandia National Laboratories

Patent applications or disclosures have been filed for Dr. Peter Van Blarigan: Free Piston Engine."

1998 Harry Lee Van Horning Memorial Award. Awarded by an SAE board of award for the single most outstanding technical contribution to SAE for 1998 in the fields of engines, fuels and combustion.

Savannah River Technology Center

Patent was awarded on composite metal hydride materials.

University of Hawaii

M.J. Antal: Catalytic Supercritical Gasification of Wet Biomass, U.S. Patent Application; Serial No. 08/414,523.

"Novel Hydrogen Storage Materials and Method of Making by Dry Homogenation"; Craig M. Jensen and Ragaiy A. Zidan; (provisional patent filled 8/98); (full patent filled, 5/99).

4.2 FY1999 Major Accomplishments

PRODUCTION

Fossil-Based Production

Demonstrated the Operation with a plasma catalyst, reducing the energy consumption to 13 MJ/kg H_2 using the conventional plasmatron. Using the novel plasmatron configuration, for both methane and diesel, the specific energy consumption was lowered below 5 MJ/kg H_2, which is lower than the energy loss due to partial oxidation. (MIT)

Demonstrated a system for hydrogen production with low CO content (~2%) with power densities of ~10 kW (H_2 HHV)/liter of reactor, or ~4 m^3/hr H_2 per liter of reactor. (MIT)

$C_{16}H_{34}$ partial oxidation is feasible, and leads to more hydrogen production than partial oxidation of diesel fuels. (ANL)

Tests on sol-gel coated metal hydride materials (composite metal hydride) show selectivity of hydrogen from CO. (SRTC)

Shakedown experiments carried out with HTC adsorbent-only have demonstrated that the CO2 adsorption system can be operated in cyclic fashion, and the CO2 adsorption capacity of the adsorbent is stable even after more than 300 adsorption/desorption cycles. (APCI)

Carried out a number of CO2/N2 breakthrough experiments with a column packed with HTC adsorbent and demonstrated: 1) the stability of the HTC CO_2 capacity after repeated CO_2 adsorption/desorption cycles, 2) fast adsorption mass transfer, 3) complete regeneration of the adsorbent with gas purge, and 4) attainment of cyclic steady-state with a repeated feed/regeneration (PSA) sequence. Conducted additional breakthrough experiments with CO2, N2 and steam and showed that the presence of steam does not affect adsorbent stability, CO_2 capacity, mass transfer rate, or regeneration requirements. (APCI)

Constructed an experimental unit [Cyclic Lifetime Unit, or CLU] to evaluate long term stability of the adsorbent and catalyst under dynamic hydrothermal process conditions and determine the effect of common natural gas impurities (H_2S, heavy hydrocarbons) on adsorbent/catalyst performance and life. (APCI)

Biomass-Based Production

The yield of gas and its composition are not significantly affected by reasonable variations in the gas phase residence time or the weight hourly space velocity within a supercritical flow reactor operating at about 700°C. (University of Hawaii)

Carbon and ash deposits accumulate primarily in the entrance region of the reactor. These deposits cause the reactor to plug after a few hours of operation. The carbon deposits are easily and quickly (<30 min) removed from the reactor by combustion in air at atmospheric pressure. The ash deposits that remain after the carbon deposits are burned out, can be easily and quickly removed with a brush. The reactor can be easily restarted after the carbon and ash deposits are removed. Initial results indicate that the reactor's performance after restarting is the same as that observed before the plug. (University of Hawaii)

Demonstrated the fluidized bed catalytic reforming process for producing hydrogen from different biomass pyrolysis liquids. The fluid bed reactor configuration proved the right approach to handling coke formation during reforming bio-oils. (NREL)

Developed a mathematical model to describe gas-liquid mass transfer in the current generation of NREL biological shift reactors; demonstrated that the experimental data are completely consistent with a biological reaction that is a gas-liquid mass transfer. (NREL)

Designed, constructed and tested a trickle-bed bioreactor (TBBR) assembly, and developed a more complex reactor model in order to more fully interpret the TBBR reactor data. (NREL)

Links with industrial and institutional partners were established aiming at scaling up the process at a regional level in Georgia. Partners include EnviroTech Inc., Scientific Carbons Inc., Clark Atlanta University, Georgia Tech, and the Cooperative Farmers Association. (NREL)

Isolated a mutant that is deficient in the uptake hydrogenase enzyme (97% less hydrogenase uptake activity than the parent). This allows the characterization of the CO-linked hydrogenase specifically without interference from other hydrogenases. (NREL)

Determined that the CO-linked hydrogenase is operative even with the simultaneous presence of oxygen. This hydrogenase is highly oxygen resistant and therefore, has great potential in scale-up process where oxygen may be present. (NREL)

RENEWABLE PRODUCTION

<u>Photo-biological Processes</u>

A library of 6,500 DNA insertional transformants was generated. Screening based on fluorescence imaging analysis resulted in the identification of (a) mutants in Chl *b* biosynthesis, having a significantly truncated Chl antenna size for photosystem-II; (b) mutants aberrant in the down-regulation of the Chl antenna size, having a conditionally truncated Chl antenna size; and (c) mutants aberrant in the up-regulation of the Chl antenna size, having an unconditionally large Chl antenna size. (University of California, Berkeley)

Successfully designed and tested a novel approach for sustained photobiological production of H_2 gas *via* the *reversible hydrogenase* pathway in the green alga *Chlamydomonas reinhardtii.* This single-organism, two-stage H_2 production method circumvents the severe O_2-sensitivity of the reversible hydrogenase by temporally separating photosynthetic O_2 evolution and carbon accumulation (Stage 1) from consumption of cellular metabolites and concomitant H_2 production (Stage 2). (University of California, Berkeley)

Developed two selective pressures and a chemochromic screening technique to, respectively, enrich for and rapidly identify stable also mutant clones that produce H_2 in the presence of controlled amounts of O_2. (NREL)

Isolated many algal mutants with improved O_2-tolerance, including two species that have O_2 I_{50}s that are 10-14 times that of the wild types. (NREL)

Developed an indirect technique to measure the photoproduction of hydrogen against atmospheres containing partial pressures of hydrogen (ORNL).

STORAGE

Produced cut nanotube segments by chemical methods which increased hydrogen uptake by more than a factor of ten on a total sample weight basis. (NREL)

Developed a simple, non-destructive, and scalable purification method that generates 98 wt % pure SWNT materials. (NREL)

Selected lithium hydride as the hydride for the slurry and light mineral oil with a dispersant as the organic carrier. (Thermo Power Corp.)

Preliminary economic analysis of the process indicates that hydrogen can be produced for $3.85 per million Btu based on a carbon cost of $1.42 per million Btu and a plant sized at 6.4 billion Btu/hr. (Thermo Power Corp.)

Performed design, analysis, and fabrication process optimization for a full-scale, two-cell, plastic-lined conformable hydrogen tank (Thiokol Propulsion)

Fabricated and hydroburst tested two full-scale tanks with cross-linked polyethylene (XLPE) liners, achieving a maximum burst pressure of 12,140 psi and one full-scale tank with polyvinylidene fluoride liners, achieving a burst pressure of 13,725 psi (Thiokol Propulsion)

Advanced Ti doped $NaAlH_4$ was developed which has >4.0 weight percent % cyclable hydrogen capacity and undergoes rapid dehydrogenation at temperatures as low as 100 ˚C. (University of Hawaii)

Ti/Zr doped $NaAlH_4$ was developed which has >4.5 weight percent % cyclable hydrogen capacity and undergoes rapid dehydrogenation at temperatures as low as 100 ˚C. (University of Hawaii)

Designed and fabricated a prototype tank which holds ~7.9 lb (3.6 kg) H2 that may attain the DOE 2000 goals of Pb*V/W ~1.85 million inches (~12% H2 by weight or 4000 Wh/kg), 700 Wh/l, and <$20/kWh (LLNL)

Large database of permeability properties acquired for polymers and laminates at pressure differentials up to 5 ksi (34.5 MPa) (LLNL)

UTILIZATION

Fuel Cells

Identified through corrosion testing several low cost alloys that performed significantly better under moderate pH conditions than 36SS. (LANL)

Demonstrated ANL composite bipolar plate technology in Plug Power cells that met or exceeded the performance of competitive composite technologies at potentially significantly lower cost. (LANL)

Demonstrated (at Plug Power) a LANL single cell with a reconfigured anode (RCA that retained over 80% of the current density of neat hydrogen operation (at 0.7 V), while using an ambient pressure reformate feed containing 50 ppm CO. (LANL)

Demonstrated very low parasitic powers (<2% not including the water recovery subsystem) for a roughly 1.5 kW half-size ambient pressure “adiabatic” stack. (LANL)

Transferred air-breather fuel cell technology to DCH, Inc. (LANL)

Scale up to larger modules (12 – 25 W) was achieved without any loss in performance compared to the "baseline" 6 – 8 W stacks. (LANL)

Numerous working demonstrations of the various "packages" of the air-breather have been performed. The typical DCH demonstration consists of simultaneously operating a camplight, portable TV and compact disk player using a single air-breather module. (LANL)

Internal Combustion Engines

Inclusion of back EMF in the finite element alternator model is critical to designing the stator geometry. The capability to include linear motion, electrical coils properly terminated and velocity profiles allows the back EMF to be accurately calculated. (SNL)

Low BTU producer gas, as generated from low sophistication, inexpensive biomass gasifiers is an excellent fuel in this combustion system due to the capability of homogeneous charge compression ignition to combust extremely lean fuel / air mixtures. Lean mixtures are a requirement with all fuels for NOx control. (SNL)

Hydrogen Safety

Produced a new sensor layout, which improves a) protection of the passive components of the sensor and b) uniformity of printed patterns on the substrate. (ORNL)

Revised sensor performance objectives to bring them into alignment with current marketing objectives. (ORNL)

Designed and built a sensor demonstration for the 1999 National Hydrogen Association meeting. The sensor was interfaced to a data acquisition system on a laptop computer. A user interface displayed the real-time hydrogen concentration and graph of the sensor response. (ORNL)

The leakage of hydrogen into a two-story building was investigated. A comparison of hydrogen leakage to helium leakage has shown the behavior of the two gases to be more similar than originally anticipated. This is good news for the development of a simple risk assessment method. (University of Miami)

Hosted ISO/TC-197 Plenary and Working Group Meetings (NHA)

TECHNOLOGY VALIDATION

Developed a hydrogen generation system that produces hydrogen from the chemical hydride slurry and water. The generator is reliable, controllable, and can supply hydrogen under moderate pressures. It produces hydrogen on demand and can be scaled to larger sizes as required. (Thermo Power Corp.)

Completed the design and fabrication of a prototype 50 kW electric-power-equivalent hydrogen generator. (Thermo Power Corp.)

ANALYSIS AND TECHNOLOGY TRANSFER

Converting from the aluminum intensive vehicles (AIV) used in previous DTI alternative vehicle comparisons to a vehicle with PNGV body characteristics does not significantly change the performance of fuel cell vehicles and hybrid electric vehicles relative to conventional vehicles -- both vehicles would have improved fuel economy and environmental emissions. However, the absolute fuel economy increases by about 27% and greenhouse gases decrease about 27% for PNGV body parameters, and the incremental cost of the direct hydrogen FCV over a conventional vehicle would decrease from $2,300 for the AIV to $1,800 for the PNGV body. (DTI)

Adding a storage battery to the stationary residential-scale fuel cell systems analyzed previously by DTI does not improve project economics. For a 3.4 kWe peak power requirement, it is estimated that a stationary fuel cell system owner would have to charge 40 4/kWh to bring a 10% real, after-tax return on investment, which is four times the average residential electrical rate in the United States. This analysis assumes that 10,000 such system are produced. (DTI)

Performed five technical evaluations during FY 1999 (Energetics)

Determined that using a low rank western coal as a carbon source for regeneration of hydrides is likely a more expensive option than using an available char. (Energetics)

Final reports were completed for the Integrated Systems activities: Analysis Tools, which contains the code details for each of the twenty-four component models developed under the activity and Design Guidelines, which includes recommendations for the optimization of existing hydrogen systems and new, promising, and desirable hydrogen systems. (NREL)

C. Elam represented the Hydrogen Agreement at the Renewable Energy Working Party (REWP) meeting in Amsterdam, the Netherlands, 26-28 May 1999. The REWP is the IEA's oversight committee for all renewable-based programs. C. Elam presented the Hydrogen Agreement's request for a five year extension to take the Agreement through June 2004. The REWP approved the request and expressed their congratulations on the recent accomplishments of the Agreement and the planned work scope for the five-year extension. Hydrogen was cited as one of the most important technologies for the coming years. (NREL)

NREL helped form the California Hydrogen Bus Coordination Committee in FY99. The Committee has adopted a charter to guide how it will function in coordinating hydrogen transit bus projects in California. (NREL)

Draft implementation plan was adopted by the NHA membership. (NHA)

Held 10th Annual U.S. Hydrogen Meeting. (NHA)

4.3 Publications and Presentations

The following publications, based on work supported by the DOE Hydrogen Program, were issued in FY1998 and 1999.

4.3.1 Research and Development

PRODUCTION

Fossil-Based Projects

Massachusetts Institute of Technology

L. Bromberg and D.R. Cohn, "System Optimization And Cost Analysis Of Plasma Catalytic Reforming Of Hydrocarbons", presented at the Fall Meeting of the American Chemical Society.

A. Rabinovich, N. Alexeev, R. Ramprasad and S. Tamhankar (http://www2.psfc.mit.edu/library/99ja/99ja017/99ja017_abs.html)

L. Bromberg, A. Rabinovich, N. Alexeev, and D.R. Cohn. "Plasma Reforming Of Diesel Fuel," (http://www2.psfc.mit.edu/ library/99ja/99ja004/99 ja004_abs.html); presented at the March meeting of the American Chemical Society.

L. Bromberg, A. Rabinovich, N. Alexeev and D.R. Cohn. "Plasma Catalytic Reforming Of Natural Gas," (http://www2.psfc.mit.edu/library/99ja/99ja016/99ja016_abs.html); presented at the March meeting of the American Chemical Society.

L. Bromberg, D.R. Cohn, K. Hadidi, A. Rabinovich and N. Alexeev, "Plasma Catalytic Reforming of Methane," *Int. Journal of Hydrogen Energy*, accepted for publication.

L. Bromberg, A. Rabinovich and D.R. Cohn, "Plasma Reformer/Fuel Cell Systems for Decentralized Energy Applications," *International Journal of Hydrogen Energy.* **22,** pp. 83 (1997).

L. Bromberg, D.R. Cohn, A. Rabinovich, C. O'Brien and S. Hochgreb, "Plasma Reforming of Methane," *Energy and Fuels,* **12**, pp. 11-18 (1998).

Air Products and Chemicals Inc.

J.R. Hufton, S. Weigel, W. Waldron, S. Nataraj, M. Rao, and S. Sircar, "Sorption Enhanced Reaction Process for Production of Hydrogen," paper presented at the 1999 U.S. DOE Hydrogen Program Review, (1999).

J.R. Hufton, S.G. Mayorga, and S. Sircar, "Sorption Enhanced Reaction Process for Hydrogen Production," *AICHE Journal*, **45**, p. 248 (1999).

J.R. Hufton, S. Mayorga, T. Gaffney, S. Nataraj, M. Rao, and S. Sircar, "Sorption Enhanced Reaction Process for Production of Hydrogen," Proceedings of the 1998 U.S. DOE Hydrogen Program Review, 693 (1998).

S. Sircar, J.R. Hufton, and S. Nataraj, "Process and Apparatus for the Production of Hydrogen by Steam Reforming of Hydrocarbon", 271PUS05829, U.S. Patent Pending (1999).

Biomass-Based Production

University of Hawaii

F. Nuessle, "Hydrogen Production from Biomass in Supercritical Flow Reactors", MSE Thesis, Dept. of Mechanical Engineering, University of Hawaii at Manoa, Honolulu, HI, 1998.

X. Xu, and M.J. Antal, "Gasification of Sewage Sludge and Other Biomass for Hydrogen Production in Supercritical Water", *Environmental Progress*, in press.

X. Xu, M.J. Antal, "Gasification of Agricultural Wastes in Supercritical Water", presented at the 1999 ACS National Meeting, Annaheim, CA, March 21.

NREL

D. Wang, S. Czernik, and E. Chornet, "Production of Hydrogen from Biomass by Catalytic Steam Reforming of Fast Pyrolysis Oils," *Energy & Fuels*, **12**, pp. 19-24 (1998).

M. Marquevich, D. Montané, D. Wang, S. Czernik, and E. Chornet, "Production of Hydrogen by Catalytic Steam Reforming of Residual Streams from Biomass Conversion Processes," *Biomass for Energy and Industry, Proceedings of the 10th European Conference and Technology Exhibition*, Wurzburg, Germany, June 1998. Kopetz, H,; Weber, T,; Palz, W,; Chartier, P.; Ferrero, G.L., Eds., pp. 1648-1651.

S. Czernik, R. French, C. Feik, and E. Chornet, "Production of Hydrogen from Hemicellulose-rich Fractions Generated through Steam Fractionation of Biomass", *Preprints of Symposia 217th ACS National Meeting*, March 21-25, 1999, Anaheim, CA. Volume 44, No. 2, pp. 240-242.

S. Czernik, R. French, C. Feik, and E. Chornet, "Production of Hydrogen from Biomass by Pyrolysis/Steam Reforming" ACS Fuel Division Meeting, New Orleans, August 1999.

S. Czernik, R. French, C. Feik, and E. Chornet, "Fluidized Bed Catalytic Steam Reforming of Pyrolysis Oil for Production of Hydrogen" *Fourth Biomass of the Americas Conference*, Oakland, CA, August 29-September 2, 1999.

M. Marquevich, S. Czernik, E. Chornet, and D. Montané, "Hydrogen from Biomass: Steam Reforming of Model Compounds of Fast Pyrolysis Oil", sent for publication in *Energy&Fuels*.

L. Garcia, R. French, S. Czernik, and E. Chornet, "Catalytic Steam Reforming of Bio-oils for the Production of Hydrogen: Effects of Catalyst Composition" prepared for publication in *Journal of Applied Catalysis*.

Renewable-Based Processes

Photo-biological Processes

ORNL

V. A. Boichenko, E. Greenbaum, and M. Seibert, "Hydrogen Production by Photosynthetic Microorganisms" in M. D. Archer and J. Barber (Eds.) *Photoconversion of Solar Energy: Volume III: Molecular to Global Photosynthesis*, Imperial College Press (in press, 1999).

E. Greenbaum and J. W. Lee, “Photosynthetic Hydrogen and Oxygen Production by Green Algae: An Overview,” in *BioHydrogen*, O. Zaborsky, Ed. pp.235-242 (1998).

National Renewable Energy Laboratory

Project was featured in the March 19, 1999 issue of "Industrial Bioprocessing Alert" an industrial newsletter.

M. Seibert, T. Flynn, D. Benson, E. Tracy and M. Ghirardi. "Prospects for Developing Algae that Produce Hydrogen under Aerobic Conditions," *Biohydrogen* (O.R. Zaborsky, ed;, J.R. Benemann, J.. Miyake, T. Matsunaga and A. San Pietro, associate eds.), Plenum Publishing Corporation, New York, N.Y., pp. 227-234 (1998).

M.L., Ghirardi, T. Flynn, M. Forestier, A. Iyer, A. Melis, P. Danielson and M. Seibert. "Generation of *C. reinhardtii* Mutants that Photoproduce H_2 from H_2O in the Presence of O_2" Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, The Netherlands, vol. III, pp. 1959-1962 (1998).

A. Melis, L. Zhang, M. Forestier, M.L. Ghirardi and M. Seibert. "Sustained Photobiological Hydrogen Gas Production upon Reversible Inactivation of Oxygen Evolution in the Green Alga *Chlamydomonas reinhardtii,*" *Plant Physiology*, submitted (1999).

T. Flynn, M.L. Ghirardi and M. Seibert. "Isolation of *Chlamydomonas* Mutants with Improved Oxygen-Tolerance," *Proc. ACS Meeting*, submitted (1999).

M. Seibert, T. Flynn and M.L. Ghirardi. "Strategies for Improving Oxygen Tolerance of Algal Hydrogen Production," *BioHydrogen 99*, submitted (1999).

M. Seibert, T.M. Flynn, M.L. Ghirardi and D.K. Benson. "A Chemochromic Sensor for Rapid Identification of Hydrogen-Producing Algal Clones," *Proc. Electrochem. Society*, submitted (1999).

M. Forestier presented a poster entitled "Attempts to clone the reversible hydrogenase of *Chlamydomonas reinhardtii* by RT-PCR" by Forestier, M., T. Flynn, M. Ghirardi and M. Seibert at the 8th Western Photosynthesis Conference, Pacific Grove, CA, January 1999.

T. Flynn presented a poster entitled "Generation of *Chlamydomonas* Mutants that Photoproduce Hydrogen from Water Under Oxygenic Conditions"by Flynn, T., M.L. Ghirardi and M. Seibert at the 8th Western Photosynthesis Conference, Pacific Grove, CA, January 1999.

Ghirardi, M. and M. Seibert made presentations at the Annual Hydrogen Program Review Meeting, Lakewood, CO, May 1999.

M. Ghirardi presented a poster entitled "Hydrogen Production by Oxygen-Tolerant *Chlamydomonas reinhardtii* Mutants" by T. Flynn, M. Ghirardi and M. Seibert at the Gordon Conference on Biochemical Aspects of Photosynthesis in New Hampshire, June 1999.

M. Seibert gave a talk entitled "Strategies for Improving Oxygen Tolerance of Algal Hydrogen Production" at the BioHydrogen 99 Workshop in Tsukuba, Japan, June 1999.

M. Ghirardi will present a paper entitled "Isolation of *Chlamydomonas* Mutants with Improved Oxygen-Tolerance" at the Hydrogen Production, Storage and Utilization Symposium being held in conjunction with the American Chemical Society National Meeting, August 1999. The paper was nominated for the Glenn Award (given for the best paper of the Fuel Chemistry Division).

Shyam S. Kocha, Don Montgomery, Mark Peterson and John A. Turner, "Photoelectrochemical Decomposition of Water Utilizing Monolithic Tandem Cells," *Solar Energy Materials and Solar Cells*, **52**, p 389 (1998).

O. Khaselev and J. A. Turner, "A Monolithic Photovoltaic-Photoelectrochemical Device for Hydrogen Production via Water Splitting," *Science,* **280**, p 425 (1998).

O. Khaselev and J. A. Turner, "Electrochemical Stability of p-$GaInP_2$ in Aqueous Electrolytes Toward Photoelectrochemical Water Splitting," *Journal of The Electrochemical Society*, **10**, p 3335-3339 (1998).

X. Gao, S. Kocha, A. J. Frank, and J. A. Turner, "Photoelectrochemical Decomposition of Water Using Modified Monolithic Tandem Cells," *International Journal Of Hydrogen Energy*, **24**, p 319-325 (1999).

J. A. Turner, "A Realizable Renewable Energy Future," *Science*, **285**, p 5428 (1999).

J. Turner, "Direct Conversion Photoelectrochemical Systems for Hydrogen Production from Sunlight and Water," *Material Research Conference*, Cancun, Mexico, September 3, 1998.

J. A. Turner, Iron Oxide Systems for Photoelectrochemical Water Splitting, (poster) 5th World Renewable Energy Congress, Florence, Italy, September, 1998.

J. Turner, "PEC Systems for Water Splitting," University of Yerevan, Yerevan, Armenia, October, 1998.

J. Turner, "Photoelectrochemical Systems for Water Splitting," February 25, 1999 and "Hydrogen Production from Sunlight and Water via Photoelectrolysis," February 26, 1999, Centro de Investigación en Energía-UNAM, Temixco, Mexico (Invited).

J. Turner, "Direct Conversion Photoelectrochemical Systems for Hydrogen Production from Sunlight and Water*,*" Charles N. Reilley award symposium (honoring Dr. Janet G. Osteryoung, Director of the Chemistry Division at the National Science Foundation), Pittcon 99 (Invited)

J. Turner, Feasibility of III-Nitride Semiconductors for Use in Hydrogen-Evolving Solar Cells. First Honda Initiation Grant Symposium, May 20, 1999. (The paper received the award for best paper in the symposium.)

J. Turner, "Solar Energy Can Supply all Our Energy Needs," *Symposium on Hydrogen B Electrochemistry and Energetics.* Trondheim, Norway, June 17, 1999 (Invited).

J. Turner, "Hydrogen Production from Water and Sunlight via Photoelectrolysis," *Fuel Cell Gordon Research Conference*. Plymouth, New Hampshire, June 27, 1999 (Invited).

P.C. Maness and P.F. Weaver, "A Potential Bioremediation Role for Photosynthetic Bacteria." *Bioremediation: Principles and Practice*, S. Sikdar (Ed.), Technomic Publishing, Lancaster, PA, pp. 149-181 (1998).

P.C. Maness and P.F. Weaver. "Three Hydrogenases of *Rhodospirillum rubrum*," in preparation for Journal of Bacteriology.

P.F. Weaver and P.-C. Maness. "Biological Conditioning of Raw Fuel Gases for Use in PEM Fuel Cells," in preparation for Applied and Environmental Microbiology.

P.F Weaver, G. Petersen, and E. Wolfrum (1998). "Quantitative Measurement of the Growth Rate and Productivity of a PHA-Producing Photosynthetic Bacterium," *AICHE Annual Meeting*, November.

University of California, Berkely

J. Neidhardt, Benemann JR, Zhang L and Melis A, "Photosystem-II repair and chloroplast recovery from irradiance stress: relationship between chronic photoinhibition, light-harvesting chlorophyll antenna size and photosynthetic productivity in *Dunaliella salina* (green algae)" *Photosynthesis*. Res. **56** pp.175-184 (1998).

A. Melis, J. Neidhardt and JR Benemann, "Maximizing photosynthetic productivity and solar conversion efficiency in microalgae by minimizing the light-harvesting chlorophyll antenna size of the photosystems" *Proceedings of the 1998 U.S. DOE Hydrogen Program Review*, April 28-30, 1998. Alexandria, Virginia. Volume I, pp. 23-41 (1998).

A. Melis, J. Neidhardt, I. Baroli and JR Benemann, "Maximizing photosynthetic productivity and light utilization in microalgae by minimizing the light-harvesting chlorophyll antenna size of the photosystems" *BioHydrogen*, (OR Zaborsky et al., eds). Plenum Publishing Corporation, New York, NY. pp. 41-52 (1998)

ML. Ghirardi, T. Flynn, A. Forestier, A. Iyer, A. Melis, P. Danielson and M. Seibert, "Generation of C. reinhardtii mutants that photoproduce H_2 from H_2O in the presence of O_2" *Photosynthesis: Mechanisms and Effects* (G Garab, ed). Kluwer Academic Publishers, The Netherlands. pp. 1959-1962 (1998).

A. Melis, J. Neidhardt and JR Benemann ,"*Dunaliella salina* (Chlorophyta) with small chlorophyll antenna sizes exhibit higher photosynthetic productivities and photon use efficiencies than normally pigmented cells" *J. Appl. Phycol*. **10**. 515-525 (1999).

JR Benemann, JC Radway and A. Melis, "Hydrogen production and biofixation of CO_2 with Microalgae" *BIOMASS, A Growth Opportunity in Green Energy and Value-added Products*, (Overend RP and Chornet E, eds). (Proc. 4th Biomass Conference of the Americas, Oakland Marriott City Center, Oakland, California, August 29 - Sept 2, 1999). Pergamon/Elsevier Science, Kidlington, Oxford, U.K. Volume 1, pp. 413-418 (1999).

A. Melis, L. Zhang, M. Forestier, GL Ghirardi and M. Seibert, "Sustained photobiological hydrogen gas production upon reversible inactivation of oxygen evolution in the green alga *Chlamydomonas reinhardtii" Plant Physiology*, accepted. (1999).

STORAGE

Carbon Structures

NREL

A.C. Dillon, T. Gennett, K.M. Jones, J.L. Alleman, P.A. Parilla, and M.J. Heben, "A Simple and Complete Purification of Single-walled Carbon Nanotube Materials" to appear in *Advanced Materials*.

A.C. Dillon, P.A. Parilla, G. Riker, J.D. Perkins, K.M. Jones, and M.J. Heben, “Effect of Pulse Width and Average Power on the Diameters of Single-Wall Carbon Nanotubes Formed by Laser Vaporization at Room Temperature” submitted to *Chemical Physics Letters*.

A.C. Dillon, J.L. Alleman, T. Gennett, K.M. Jones, P.A. Parilla, and M.J. Heben, "Combined Effect of Synthesis Temperature and Laser Energy Density on the Diameter Distributions of Single-wall Carbon Nanotubes" manuscript in preparation.

T. Gennett, A.C. Dillon, J.L. Alleman, K.M. Jones, and M.J. Heben, "Formation of Single-Wall Carbon Nanotube Superbundles" manuscript in preparation.

T. Gennett, A.C. Dillon, J.L. Alleman, K.M. Jones, P.A. Parilla, and M.J. Heben, "Synthesis of Homogeneous Diameter Single-wall Carbon Nanotubes by Laser Vaporization" manuscript in preparation.

M.J. Heben, “Invited Presentation, Hydrogen Storage Activities at NREL”, 10th Annual meeting of the U.S. National Hydrogen Association, Vienna, VA, April 9, 1999.

M.J. Heben: Invited Participation in the Gordon Research Conference on Hydrogen : Metal Systems, New England College, Henniker, NH, July 19-23, 1999.

M.J. Heben: Invited Presentation, The Research Association for the Development and Application of Metal-Hydrogen Systems in Japan, Kogakuin University, Tokyo, Japan, October 2, 1998.

A.C. Dillon, "The Production Of Single-Wall Carbon Nanotubes With Specific Diameters By Varying Pulsed Laser Vaporization Synthesis Parameters" *1999 Fall Meeting of the Materials Research Society*, Boston, MA, December 1, 1998.

M.J. Heben: “Carbon Nanotube Materials for Hydrogen Storage” Meeting of the Experts of Annex 12 of the International Energy Agency” Kogakuin University, Tokyo, Japan, October 1, 1998.

M.J. Heben, “Carbon Materials and Hydrogen Storage” presented at the Meeting of the Experts of Annex 12 of the International Energy Agency, New England College, Henniker, NH, July 20-21, 1999.

Metal Hydrides

Thermo Power Corporation

R. W. Breault, J. Rolfe, and A. McClaine, “Hydrogen Transmission/Storage with a Chemical Hydride/Organic Slurry”, *9th Canadian Hydrogen Conference*, Vancouver, British Columbia, 7-10 Feb. 1999.

R. W. Breault, J. Rolfe, and A. McClaine, “Hydrogen for the Hydrogen Economy”, *24th Coal Utilization and Fuel Systems Conference*, Clearwater, FL, 8-11 March 1999.

R. W. Breault, and J. Rolfe, “Chemical Hydride Hydrogen Storage Canisters for DOD Fuel Cell Applications”, *10th National Hydrogen Association Conference*, Tysons Corner, VA, 7-9 April 1999.

R. W. Breault, C. Larson, and J. Rolfe, “Hydrogen for a PEM Fuel Cell Vehicle Using a Chemical-Hydride Slurry”, *10th National Hydrogen Association Conference*, Tysons Corner, VA, 7-9 April 1999.

R. W. Breault, A. W. McClaine, J. Rolfe, and C. Larsen, "Sustainable Hydrogen for the Hydrogen Economy", *218th American Chemical Society Division of Fuel Chemistry Symposia*, New Orleans, LA, August 22-26,1999, Volume 44, No. 4.

University of Hawaii

R. A. Zidan, S. Takara, A. G. Hee, and C. M. Jensen ,"Hydrogen Cycling Behavior of Zirconium and Titanium-Zirconium Doped Sodium Aluminum Hydride."; *Journal of Alloys and Compounds*, **285**. p 119 (1999).

C. M. Jensen, R. Zidan, N. Mariels, A. Hee, and C. Hagen, "Advanced Titanium Doping of Sodium Aluminum Hydride: Segue to a Practical Hydrogen Storage Material?" *International Journal of Hydrogen Energy*, **24**. 461 (1999)

F. Liu, E. B. Pak, B. Singh, C. M. Jensen, and A. S. Goldman, "Dehydrogenation of n-Alkanes Catalyzed by Iridium Pincer Complexes: Regioselective Formation of Alpha-Olefins" *J. Am. Chem. Soc.* ,**121**. 4086 (1999) (subject of *Chemical and Engineering News* feature article 7/5/99)

C. M. Jensen, "Catalytic Dehydrogenation of Sodium Aluminum Hydride" *Special Symposium of the Research Association for the Development and Application of Metal-Hydrogen Systems*, Tokyo, Japan, October 2, 1998.

R.A. Zidan, S. Takara, A.G. Hee, and C.M. Jensen (presented by G. Sandrock), "Hydrogen Cycling Behavior of Zirconium and Titanium-Zirconium Doped Sodium Aluminum Hydride." *International Symposium on Metal-Hydrogen Systems*, Hangzhou, China, October 4-9, 1998.

C. M. Jensen, "Catalytically Enhanced Sodium Aluminum Hydride as a Hydrogen Storage Material" invited seminar, Morton International Inc.; October 27, 1998.

E. B. Pak, C. Hagen, and C. M. Jensen, "Regioselective Dehydrogenation of Linear Alkanes to Alpha Olefins by An Iridium P-C-P Pincer Complex" *217th American Chemical Society National Meeting*, Anaheim, California; March 21-25, 1999.

C. M. Jensen, "Catalytically Enhanced Sodium Aluminum Hydride as a Hydrogen Storage Material" research success story award presentation, U.S. Department of Energy Hydrogen Technical Advisory Panel Meeting, Vienna, Virginia; April 6, 1999.

R. A. Zidan, "Catalytically Enhanced Aluminum Hydrides: Practical Hydrogen Storage Materials?" presented at the Gordon Research Conference on Hydrogen-Metal Systems; Henniker, New Hampshire 7/99.

C. M. Jensen, R. Zidan; S. Takara; A. Hee, K. Magnuson, and C. Hagen, "Catalytically Enhanced Sodium Aluminum Hydride as a Hydrogen Storage Material" *Symposium on Hydrogen Production, Storage, and Utilization, 218th American Chemical Society National Meeting*, New Orleans, Louisiana; August 22-27, 1999.

D. Morales-Morales, W. Chen, and C.M. Jensen, "Catalytic Production of Imines through the Dehydrogenation of Secondary Amines by a Hydrido PCP Pincer Complex" *218th American Chemical Society National Meeting*, New Orleans, Louisiana; August 22-27, 1999.

Physical Storage

Thiokol Propulsion

R. K. Kunz, R. P. Golde, B. M. McQuivey, "High Pressure Conformable Hydrogen Storage for Fuel Cell Vehicles," *Proceedings, 10th Annual U.S. Hydrogen Meeting and Exhibition*, Vienna, VA, April 7-9, 1999, sponsored by National Hydrogen Association.

R. P. Golde, R. K. Kunz, M. J. Warner, "The Shape of Things to Come," *SAMPE Journal*, March/April (1999)

Lawrence Livermore National Laboratory

F. Mitlitsky, A.H. Weisberg, P.H. Carter, M.D. Dittman, and B. Myers, R.W. Humble, and J.T. Kare, "Water Rocket – Electrolysis Propulsion and Fuel Cell Power" AIAA-99-4609, AIAA Space Technology Conference, Albuquerque, NM, September 28-30 (1999).

F. Mitlitsky and A.H. Weisberg, "Water-Based Spacecraft", invited presentation, JASONs Program Office, Space Architecture Panel, La Jolla, CA, July 12 (1999).

F. Mitlitsky, B. Myers, A.H. Weisberg, and A. Leonida, "Applications and Development of High Pressure PEM Systems", invited presentation, Portable Fuel Cells International Conference, Lucerne, Switzerland, June 21-24 (1999); UCRL-JC-134539.

F. Mitlitsky, B. Myers, A.H. Weisberg, T.M. Molter, and W.F. Smith, "Reversible (Unitized) PEM Fuel Cell Devices" invited presentation, Portable Fuel Cells International Conference, Lucerne, Switzerland, June 21-24 (1999), and Feature Article, Fuel Cells Bulletin, Number 11, August (1999); UCRL-JC-134538.

F. Mitlitsky, A.H. Weisberg, and B. Myers, "Vehicular Hydrogen Storage Using Lightweight Tanks (Regenerative fuel cell systems)," DOE Hydrogen Program Annual Review, Lakewood, CO, May 4-6 (1999); UCRL-JC-134540.

J.T. Kare, F. Mitlitsky, and A.H. Weisberg, "Preliminary Demonstration of Power beaming with Non-coherent Laser Diode Arrays" *Space Technology and Applications International Forum (STAIF-99),* Albuquerque, NM, January 31 - February 4 (1999): UCRL-JC-133428.

F. Mitlitsky, "Water Rocket Technologies" invited presentation, US Embassy, Paris, France, December 10-11 (1998); UCRL-MI-132628 Rev 1.

F. Mitlitsky, B. Myers, A.H. Weisberg, and T.M. Molter, "Unitized regenerative fuel cell systems" *Fuel Cell Seminar*, Palm Springs, CA, November 16-19 (1998); UCRL-JC-130198 (paper) and UCRL-MI-130198 (viewgraphs).

F. Mitlitsky, P.H. Carter, M.D. Dittman, R.W. Humble, J.T. Kare, B. Myers, and A.H. Weisberg, "Water Rocket Design Trade Analysis" October 29 (1998); and briefing at AFRL Edwards AFB on Nov. 6 (1998).

J.F. McElroy, R.W. Humble, W.A. de Groot, S.R. Oleson, F. Mitlitsky, A.H. Weisberg, B. Myers, and P.H. Carter II, "Unitized Electrolysis Propulsion and Fuel Cell Power for Selected Satellite Missions" *33rd Intersociety Energy Conversion Engineering Conference (IECEC),* Colorado Springs, CO, August 2-6, 1998 (IECEC-98-339).

F. Mitlitsky, B. Myers, and A.H. Weisberg, "Regenerative Fuel Cell Systems R&D" *DOE Annual Hydrogen Program Peer Review*, Alexandria, VA, April 28-30 (1998), and invited presentation, Joint DOE/EPRI/GRI Workshop on Fuel Cell Technology, San Francisco, CA, May 18-20 (1998); UCRL-JC-131087.

P.H. Carter II, F. Mitlitsky, A.H. Weisberg, J.C. Whitehead, and R.W. Humble, "Design Trade Space for a Mars Ascent Vehicle for a Mars Sample Return Mission" IAA Conference on Low-Cost Planetary Missions, Pasadena, CA, April 27-May 1 (1998); UCRL-JC-130277.

F. Mitlitsky, A.H. Weisberg, and B. Myers, "Regenerative Fuel Cell Systems**"** *Energy & Fuels*, 12 (1), 56-71, January 12 (1998); UCRL-JC-128267 Rev 1; http://pubs.acs.org/isubscribe/journals/enfuem/jtext.cgi?enfuem/12/i01/html/ef970151w.html

UTILIZATION

Enabling Projects

Sandia National Laboratories

P. Van Blarigan, "Advanced Hydrogen Fueled Internal Combustion Engines", *Energy & Fuels*, **12**. 72 – 77 (1998)

P. Van Blarigan, et al, "Homogeneous Charge Compression Ignition with a Free Piston: A New Approach to Ideal Otto Cycle Performance", SAE 982484, October 1998.

Hydrogen Safety

Oak Ridge National Laboratory

B. S. Hoffheins, L. C. Maxey, W. Holmes, Jr., R. J. Lauf, C. Salter, and D. Walker, "Development Of Low Cost Sensors For Hydrogen Safety Applications," *Proceedings of the 1999 U.S. DOE Hydrogen Program Review*, in publication.

B.S., Hoffheins, J.E. Rogers, R. J. Lauf, D. P. Haberman, and C.M. Egert. "Low-Cost Hydrogen Sensor: Technology Maturation Progress" *Proceedings of the 1998 U.S. DOE Hydrogen Program Review*. NREL/CP-570-225315. Volume I. August 1998.

University of Miami

M. R. Swain, J. Schriber, and M. N. Swain, "Comparison of Hydrogen, Natural Gas, Liquified Petroleum Gas, and Gasoline Leakage in a Residential Garage" *Energy and Fuels*, January 1998, pp 83-89

One of eight authors of "Hydrogen Source Book" written by Hydrogen Safety Working Group convened by NREL

The Hydrogen Technical Advisory Panel (HTAP) awarded the Safety Analysis work at the University of Miami their Research Excellence Award on March 3, 1998 at the 9th Annual US Hydrogen Meeting

M.R. Swain, E.S. Grilliot, M.N. Swain, "Experimental Verification of a Hydrogen Risk Assessment Method", published by the American Chemical Society in Chemical Health and Safety, Vol 6, No. 3, May/June 1999, pp 28-32

M.R. Swain, E.S. Grilliot, M.N. Swain, “The Application of a Hydrogen Risk Assessment Method” presented at the 218th American Chemical Society National Meeting in New Orleans, Louisiana, August 22-24, 1999

4.3.2 Technology Validation

Hydrogen Infrastructure

Filling up with Hydrogen 2000 – Stuart Energy Systems

M. Fairlie, “Hydrogen Fuels: Tackling Transportation Green House Emissions” *Energy and Environment Conference*, Toronto, Nov 1998.

D. Martin, “The Stuart Fuel Appliance – “ A Plug and Play Approach to Hydrogen Supply” *Proceedings of the 10th Annual U.S. Hydrogen Meeting*, Vienna, Virginia, April 1999. pp 547-573.

A. Stuart, “Stuart Fuel Appliances: Connecting Electricity to Fuel Markets”, *Canadian Fllet Maintenance Seminar*, Windsor Ont., April 1999.

M. Fairlie, P. Scott, A.T.B.S. Stuart, “Electrolytic Hydrogen Re-Fuelers for Fleet and Home Use”, Society Automotive Engineers, 99-01-2898, Costa Mesa, CA, August 1999.

Thermo Power Corporation

R. W. Breault, J. Rolfe, and A. McClaine, “Hydrogen Transmission/Storage with a Chemical Hydride/Organic Slurry” *9th Canadian Hydrogen Conference*, Vancouver, British Columbia, 7-10 Feb. 1999

R. W. Breault, J. Rolfe, and A. McClaine, “Hydrogen for the Hydrogen Economy” *24th Coal Utilization and Fuel Systems Conference*, Clearwater, FL, 8-11 March 1999

R. W. Breault, and J. Rolfe, “Chemical Hydride Hydrogen Storage Canisters for DOD Fuel Cell Applications” *10th National Hydrogen Association Conference*, Tysons Corner, VA, 7-9 April 1999

R. W. Breault, C. Larson, and J. Rolfe, “Hydrogen for a PEM Fuel Cell Vehicle Using a Chemical-Hydride Slurry” *10th National Hydrogen Association Conference*, Tysons Corner, VA, 7-9 April 1999

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4.3.3 Analysis and Technology Transfer

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